

(130)

New search

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-5.58	-5.58

STN INTERNATIONAL LOGOFF AT 09:38:09 ON 13 AUG 2002

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
 NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
 NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
 NEWS 4 Apr 09 ZDB will be removed from STN
 NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
 NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
 NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
 NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
 NEWS 9 Jun 03 New e-mail delivery for search results now available
 NEWS 10 Jun 10 MEDLINE Reload
 NEWS 11 Jun 10 PCTFULL has been reloaded
 NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
 NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
 saved answer sets no longer valid
 NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
 NEWS 15 Jul 30 NETFIRST to be removed from STN
 NEWS 16 Aug 08 CANCERLIT reload
 NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
 NEWS 18 Aug 08 NTIS has been reloaded and enhanced
 NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
 now available on STN
 NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
 NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
 NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
 NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
 NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
 NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
 NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA

 NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
 CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
 AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
 NEWS HOURS STN Operating Hours Plus Help Desk Availability
 NEWS INTER General Internet Information
 NEWS LOGIN Welcome Banner and News Items
 NEWS PHONE Direct Dial and Telecommunication Network Access to STN
 NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus *

FILE 'HOME' ENTERED AT 09:21:28 ON 19 SEP 2002

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n) :

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE
ENTRY | TOTAL
SESSION |
|----------------------|---------------------|------------------|
| FULL ESTIMATED COST | 1.26 | 1.26 |

FILE 'REGISTRY' ENTERED AT 09:24:47 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2002 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3
DICTIONARY FILE UPDATES: 17 SEP 2002 HIGHEST RN 452274-20-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 30, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

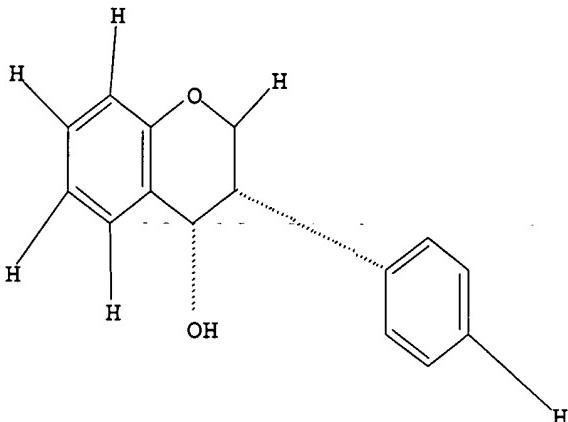
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 09889701a.str

L1 STRUCTURE UPLOADED

Golam Shameem

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 09:25:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 672 TO ITERATE

100.0% PROCESSED 672 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 11885 TO 14995
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 09:25:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 13644 TO ITERATE

100.0% PROCESSED 13644 ITERATIONS
SEARCH TIME: 00.00.01

28 ANSWERS

L3 28 SEA SSS FUL L1

| | | |
|----------------------|------------|---------|
| => FIL CAPLUS | SINCE FILE | TOTAL |
| COST IN U.S. DOLLARS | ENTRY | SESSION |
| FULL ESTIMATED COST | 140.66 | 141.92 |

FILE 'CAPLUS' ENTERED AT 09:25:53 ON 19 SEP 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Golam Shameem

09/19/2002

Connecting via Winsock to STN

130

New search

Welcome to STN International! Enter x:x

LOGINID:ssspta1626gms

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * Welcome to STN International * * * * * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
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saved answer sets no longer valid
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NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 09 JAPIO to be reloaded August 18, 2002

NEWS EXPRESS February 1 CURRENT WINDOWS VERSION IS V6.0d,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 05 FEBRUARY 2002
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NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * STN Columbus * * * * * * * * * * *

FILE 'HOME' ENTERED AT 09:31:56 ON 13 AUG 2002

Golam Shameem

=>

Uploading

THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE

Do you want to switch to the Registry File?

Choice (Y/n) :

Switching to the Registry File...

Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|----------------------|------------------|---------------|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'REGISTRY' ENTERED AT 09:32:15 ON 13 AUG 2002

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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STRUCTURE FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

DICTIONARY FILE UPDATES: 12 AUG 2002 HIGHEST RN 443729-39-3

TSCA INFORMATION NOW CURRENT THROUGH January 7, 2002

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Calculated physical property data is now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:

<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>

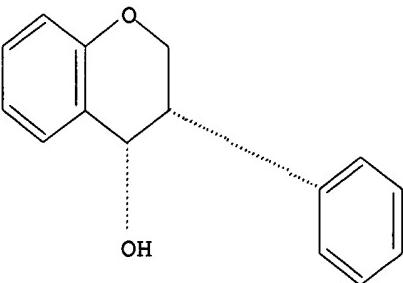
Uploading 09889701.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

Golam Shameem

=> s 11
 SAMPLE SEARCH INITIATED 09:32:32 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 604 TO ITERATE

100.0% PROCESSED 604 ITERATIONS 11 ANSWERS
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 10606 TO 13554
 PROJECTED ANSWERS: 21 TO 417

L2 11 SEA SSS SAM L1

=> FIL CAPLUS
 COST IN U.S. DOLLARS SINCE FILE TOTAL
 FULL ESTIMATED COST ENTRY SESSION
 0.38 0.59

FILE 'CAPLUS' ENTERED AT 09:32:42 ON 13 AUG 2002
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
 COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 13 Aug 2002 VOL 137 ISS 7
 FILE LAST UPDATED: 12 Aug 2002 (20020812/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 11
REGISTRY INITIATED
 Substance data SEARCH and crossover from CAS REGISTRY in progress...
 Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 09:32:47 FILE 'REGISTRY'
 SAMPLE SCREEN SEARCH COMPLETED - 604 TO ITERATE

100.0% PROCESSED 604 ITERATIONS
 SEARCH TIME: 00.00.01

11 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**
 PROJECTED ITERATIONS: 10606 TO 13554
 PROJECTED ANSWERS: 21 TO 417

L3 11 SEA SSS SAM L1

L4 8 L3

=> s l3/prep
 8 L3
 2897488 PREP/RL
 L5 5 L3/PREP
 (L3 (L) PREP/RL)

=> s l3/proc
 8 L3
 3189134 PROC/RL
 L6 0 L3/PROC
 (L3 (L) PROC/RL)

=> s l5 and hydrogenation
 147967 HYDROGENATION
 1893 HYDROGENATIONS
 148239 HYDROGENATION
 (HYDROGENATION OR HYDROGENATIONS)
 L7 2 L5 AND HYDROGENATION

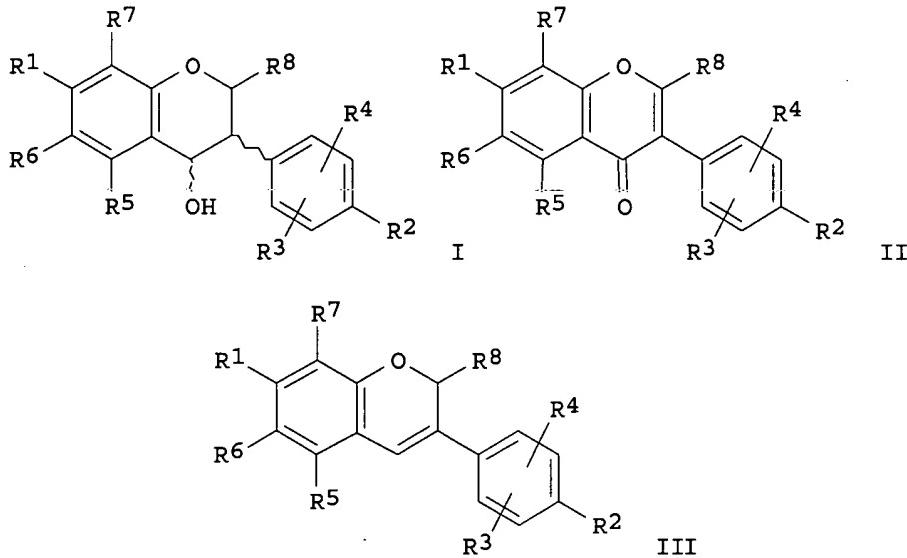
=> d ibib abs hitstr 17

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:592710 CAPLUS
 DOCUMENT NUMBER: 133:177059
 TITLE: Preparation of isoflavone derivatives
 INVENTOR(S): Heaton, Andrew; Kumar, Naresh
 PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|--|----------|-----------------|----------|
| WO 2000049009 | A1 | 20000824 | WO 2000-AU103 | 20000215 |
| W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |

BR 2000008222 A 20011030 BR 2000-8222 20000215
 EP 1153020 A1 20011114 EP 2000-904727 20000215
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, SI, LT, LV, FI, RO
 NO 2001003945 A 20010814 NO 2001-3945 20010814
 PRIORITY APPLN. INFO.: AU 1999-8685 A 19990215
 WO 2000-AU103 W 20000215

OTHER SOURCE(S): MARPAT 133:177059
 GI



AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH₂, NO₂, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prep'd. Thus, daidzein diacetate was prep'd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

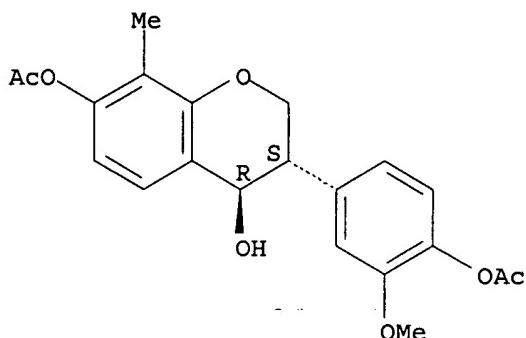
IT 288266-89-7P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (**Preparation**); RACT (Reactant or reagent)
 (prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



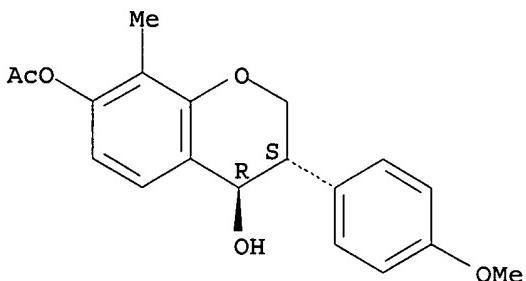
IT 288266-88-6P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



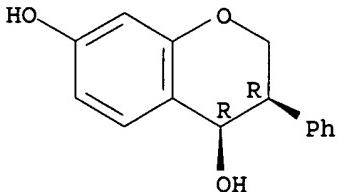
IT 288267-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

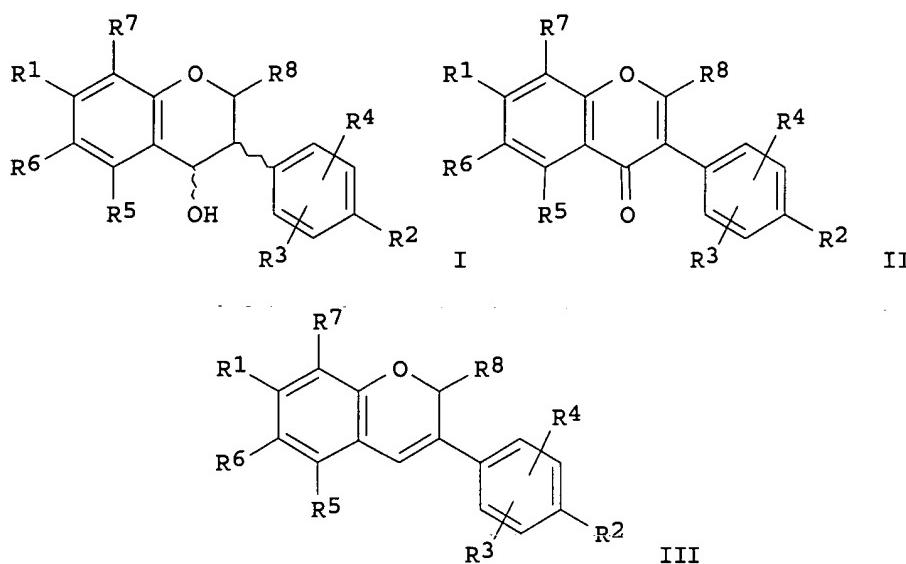
14

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 15

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:592710 CAPLUS
 DOCUMENT NUMBER: 133:177059
 TITLE: Preparation of isoflavone derivatives
 INVENTOR(S): Heaton, Andrew; Kumar, Naresh
 PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|-------------------|----------|-----------------|------------|
| WO 2000049009 | A1 | 20000824 | WO 2000-AU103 | 20000215 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| BR 2000008222 | A | 20011030 | BR 2000-8222 | 20000215 |
| EP 1153020 | A1 | 20011114 | EP 2000-904727 | 20000215 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | | |
| NO 2001003945 | A | 20010814 | NO 2001-3945 | 20010814 |
| PRIORITY APPLN. INFO.: | | | AU 1999-8685 | A 19990215 |
| | | | WO 2000-AU103 | W 20000215 |
| OTHER SOURCE(S): | MARPAT 133:177059 | | | |
| GI | | | | |



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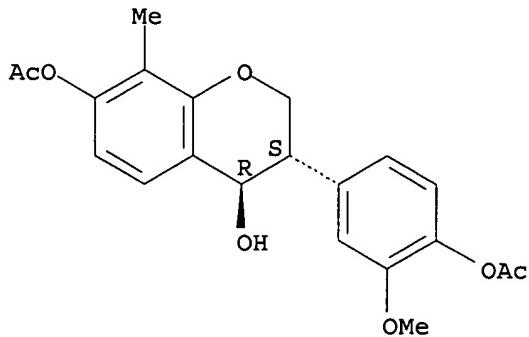
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(prep'n. of isoflavone derivs.)

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Relative stereochemistry.



IT 288266-88-6P

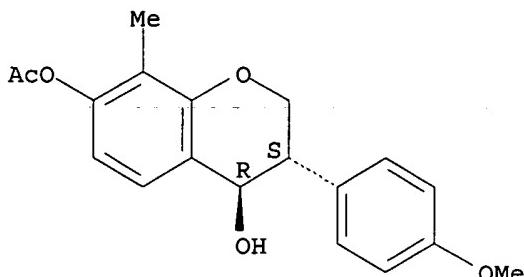
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reagent); USES (Uses)
 (prep. of isoflavone derivs.)

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Relative stereochemistry.



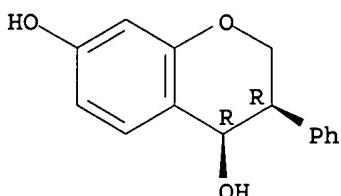
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Relative stereochemistry.



REFERENCE COUNT:

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=> d ibib abs hitstr 15 tot

L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:592710 CAPLUS

DOCUMENT NUMBER: 133:177059

TITLE: Preparation of isoflavone derivatives

INVENTOR(S): Heaton, Andrew; Kumar, Naresh

PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia

SOURCE: PCT Int. Appl., 55 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

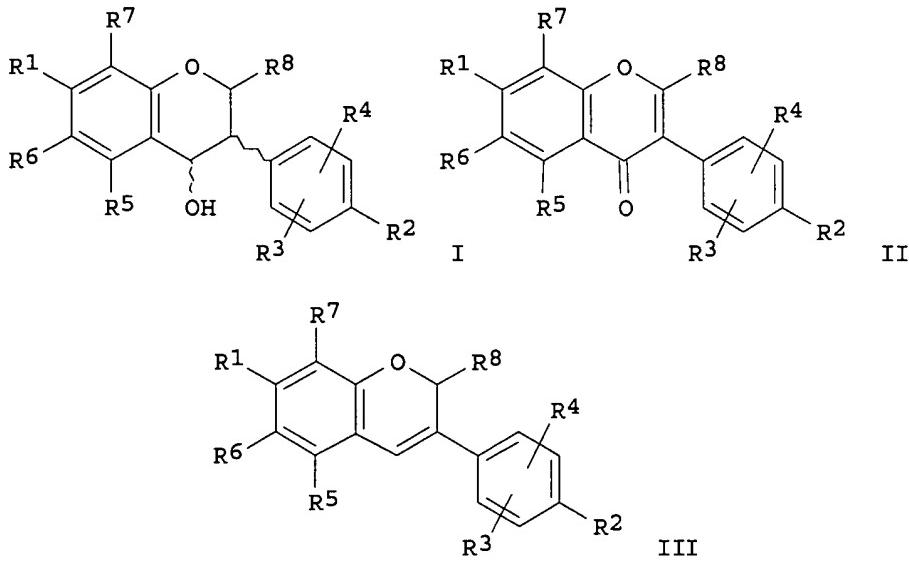
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|-------|-------|-----------------|-------|
| ----- | ----- | ----- | ----- | ----- |

| | | | |
|--|-------------|----------------|------------|
| WO 2000049009 | A1 20000824 | WO 2000-AU103 | 20000215 |
| W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL,
IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA,
MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI,
SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| BR 2000008222 | A 20011030 | BR 2000-8222 | 20000215 |
| EP 1153020 | A1 20011114 | EP 2000-904727 | 20000215 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, SI, LT, LV, FI, RO | | | |
| NO 2001003945 | A 20010814 | NO 2001-3945 | 20010814 |
| PRIORITY APPLN. INFO.: | | AU 1999-8685 | A 19990215 |
| | | WO 2000-AU103 | W 20000215 |

OTHER SOURCE(S) : MARPAT 133:177059
GI



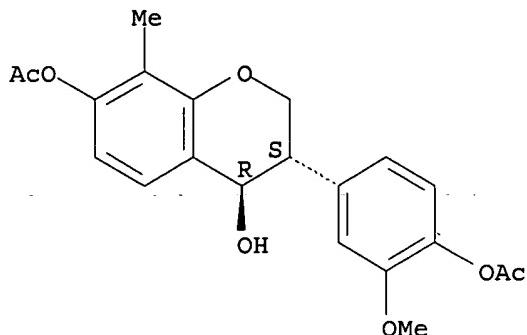
AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH₂, NO₂, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prep'd. Thus, daidzein diacetate was prep'd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the hydrogenation of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflav-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

IT 288266-89-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(prepn. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



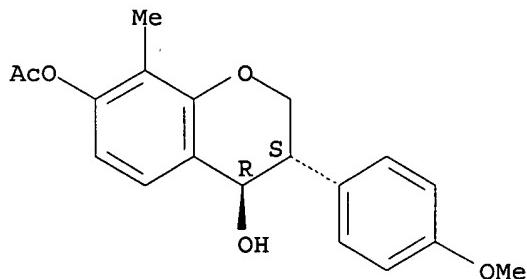
IT 288266-88-6P

RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



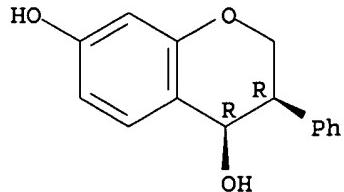
IT 288267-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



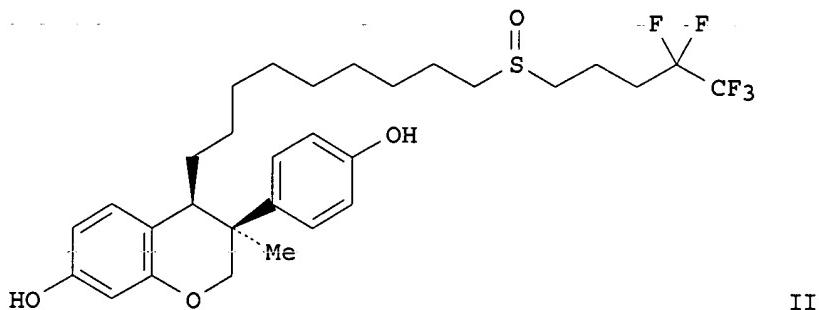
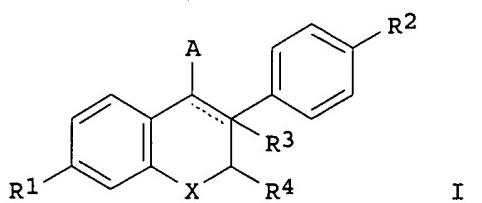
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:402432 CAPLUS
 DOCUMENT NUMBER: 129:81667
 TITLE: Novel benzopyran and thiochroman derivatives useful as antiestrogens
 INVENTOR(S): Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-hwa
 PATENT ASSIGNEE(S): C & C Research Laboratories, S. Korea; Jo, Jae Chon; Park, Sung Dae; Lim, Hyun Suk; Kim, Ju Su; Kim, Sung Jin; Morikawa, Kazumi; Kanbe, Yoshitake; Nishimoto, Masahiro; Kim, Myung-Hwa
 SOURCE: PCT Int. Appl., 125 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|------------|
| WO 9825916 | A1 | 19980618 | WO 1997-KR265 | 19971213 |
| W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG | | | | |
| AU 9854134 | A1 | 19980703 | AU 1998-54134 | 19971213 |
| AU 722089 | B2 | 20000720 | | |
| EP 944613 | A1 | 19990929 | EP 1997-947971 | 19971213 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | | | | |
| CN 1244863 | A | 20000216 | CN 1997-181472 | 19971213 |
| JP 2000507620 | T2 | 20000620 | JP 1998-526521 | 19971213 |
| JP 3251946 | B2 | 20020128 | | |
| US 6153768 | A | 20001128 | US 1999-319616 | 19990608 |
| PRIORITY APPLN. INFO.: | | | KR 1996-65301 | A 19961213 |
| | | | KR 1997-26915 | A 19970624 |
| | | | WO 1997-KR265 | W 19971213 |

OTHER SOURCE(S): MARPAT 129:81667

GI



AB The invention relates to novel benzopyran derivs. having anti-estrogenic activity. More specifically, the invention relates to novel benzopyran and thiochroman derivs. I and pharmaceutically acceptable salts thereof [in which the dashed line = optional pi bond; R1, R2 = H, OH, or OR; R = acyl or alkyl; R3 = H, alkyl, haloalkyl, or null when R3 is absent; R4 = H or alkyl; A = $(CH_2)_mSONR_5$, $C_6H_4O(CH_2)_mNR_6R_7$, $(CH_2)_mSON(CH_2)pNR_6R_7$; R5, R6, and R7 = H, alkyl, haloalkyl, alkenyl, or haloalkenyl; or NR6R7 = 4- to 8-membered heterocyclic ring which can be substituted with R5; X = O, S, or NR8; R8 = H or alkyl; m = 2-15; n = 0-2; and p = 0-4]. Also disclosed are a prepn. process, and antiestrogenic pharmaceutical compns. which contains I as an active component. Examples include over 80 syntheses and 4 bioassays. For example, compd. II was prep'd. by a 7-step sequence involving: (1) double-O-methoxymethylation and 3-methylation of 7-hydroxy-3-(4-hydroxyphenyl)-2,3-dihydro-4H-benzopyran-4-one (66%), (2) 4-alkynylation with HC.tpbond.C(CH₂)₇OSiMe₂CMe₃ (100%), (3) desilylation (33%), O-tosylation (88%), thioetherification (97%), deprotection of OH groups (66%), and S-oxidn. with NaIO₄ (73%). The antiestrogenic and MCF-7 cell growth-inhibiting activities of II were comparable or superior to the related antiestrogen ZM-189154, and the side effect of decreased bone mineral d. in II was not only reduced but to some extent reversed.

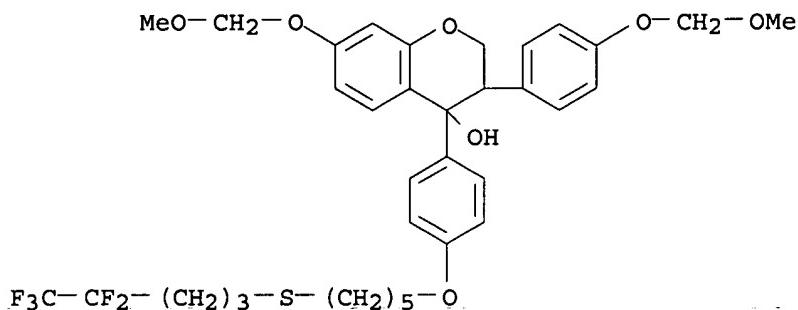
IT 209324-98-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prep'n. of benzopyran and thiochroman derivs. as antiestrogens)

RN 209324-98-1 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-7-(methoxymethoxy)-3-[4-(methoxymethoxy)phenyl]-4-[4-[[5-[(4,4,5,5,5-pentafluoropentyl)thio]pentyl]oxy]phenyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:148589 CAPLUS

DOCUMENT NUMBER: 104:148589

TITLE: The chemistry of the 'insoluble red woods'. Part 16.
Some further observations on the condensation of

isoflavylium salts with 1,3-diphenylpropenes

AUTHOR(S): Afonya, Theophilus C. A.; Epelle, Faithwin B. M.; Osman, Soad A. A.; Whalley, W. Basil

CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK

SOURCE: J. Chem. Res., Synop. (1985), (10), 305

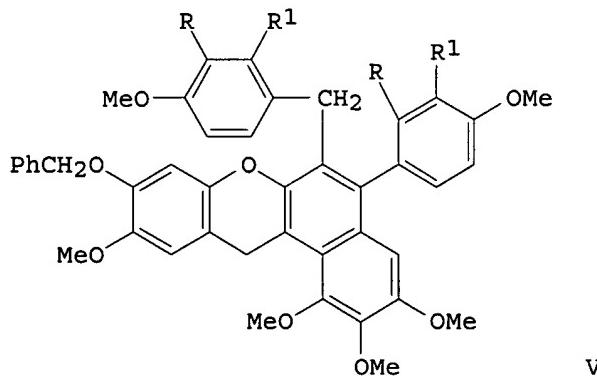
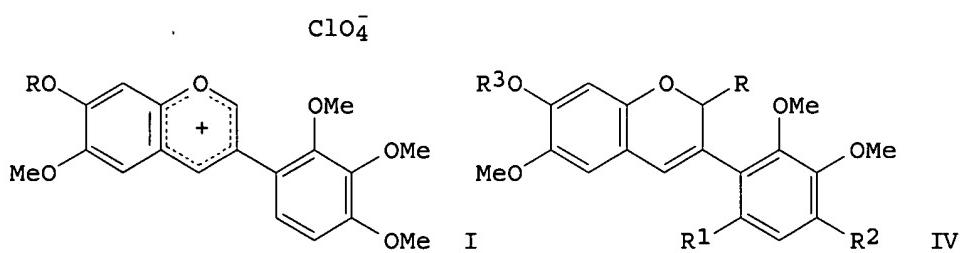
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:148589

GI

AB Condensation of isoflavylium perchlorate I ($R = \text{CH}_2\text{Ph}$) (II) with

Golam Shameem

3,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-2,4 (III) in refluxing MeCN for 3 h gave isoflavene IV (R = R1 = H, R2 = OMe, R3 = CH2Ph) and benzoxanthene V (R = H, R1 = OMe). Similar reaction of II with 2,4-(MeO)2C6H3CH:CHCH2C6H3(OMe)2-3,4 (VI) gave isoflavene IV (R = R2 = OMe, R1 = H; R = R2 = H, R1 = OMe; R3 = CH2Ph) and benzoxanthene V (R = OMe, R1 = H). Analogous reaction of I (R = Me) with III or VI gave only the isoflavene IV (R = R2 = OMe, R1 = H, R3 = Me). The preps. of the starting materials are reported.

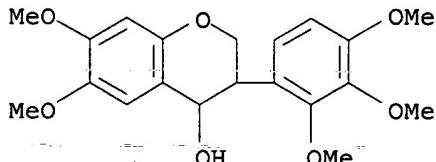
IT 100753-48-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)-(9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:476524 CAPLUS

DOCUMENT NUMBER: 75:76524

TITLE: Reactions of isoflavanones with Grignard reagents.
Synthesis of estrogenic and antiestrogenic active
isoflavanoids

AUTHOR(S): Irmscher, Klaus; Borck, Joachim

CORPORATE SOURCE: Chem. Forsch. E. Merck, Darmstadt, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1971), 744, 164-77

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Grignard reaction of isoflavanones or 2-ethyl-7-methoxyisoflavanones (I) gave 4-aryl-4-isoflavanols or 2-ethyl-7-methoxy-4-aryl-4-isoflavanols (II), resp., which were dehydrated to 4-aryl-3-isoflavenes. Depending on the reaction conditions, the constitution of the isoflavanone, and the Grignard reagent, the C-2 atom of the isoflavanone was also attached in some cases to give .beta.-aryl-.alpha.-phenyl-2-hydroxypropiophenones with ring opening. The mechanism of the ring opening involving an .alpha.-methylene ketone was discussed.

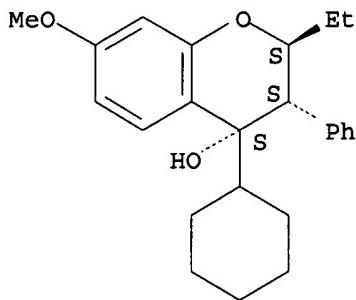
IT 33103-17-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 33103-17-2 CAPLUS

CN 4-Isoflavanol, 4-cyclohexyl-2-ethyl-7-methoxy-, stereoisomer (8CI) (CA INDEX NAME)

Relative stereochemistry.



L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1967:28657 CAPLUS
 DOCUMENT NUMBER: 66:28657
 TITLE: 3,4-Diaryl-4-chromanols and 3,4-diaryl-3-chromenes
 PATENT ASSIGNEE(S): Merck, E., A.-G.
 SOURCE: Neth. Appl., 26 pp.
 CODEN: NAXXAN
 DOCUMENT TYPE: Patent
 LANGUAGE: Dutch
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|-------|----------|-----------------|-------|
| NL 6517021 | ----- | 19660704 | ----- | ----- |

PRIORITY APPLN. INFO.: DE 19650102
 GI For diagram(s), see printed CA Issue.
 AB The title compds. are prep'd. by condensation of 3-aryl-4-chromanones with organo-metallic compds. followed by dehydration. A soln. of 0.66 g. I (R = R₁ = H) (IV) in 30 ml. abs. C₆H₆ is dropped to a soln. of p-MeOC₆H₄MgBr (from 2.2 g. p-MeOC₆H₄Br and 0.23 g. Mg) in abs. Et₂O, the Et₂O distd., and the mixt. refluxed 16 hrs., cooled, decompd. with 100 ml. 10% HCl, and the C₆H₆ layer sped. to yield II (R = R₁ = H, R₂ = MeO), m. 144-5.degree. (CHCl₃-Et₂O). Likewise, the following II are prep'd. (R, R₁, R₂, and m.p. given): H, H, H, 127-31.degree. (V); Et, H, H, 121-3.degree.; H, MeO, H, 151-2.degree.; Et, MeO, H, 158.degree. and 105.degree. (2 isomers); Et, MeO, MeO, 105-6.degree.; H, H, PhCH₂O, 122-3.degree. (VI); Et, MeO, PhCH₂O, 126.degree. and 137.degree. (2 isomers). To a soln. of IV (0.68 g.) in 30 ml. abs. C₆H₆ is added dropwise a soln. of PhLi (4 millimoles) in Et₂O. After the same treatment as above V is isolated; when the mixt. is heated 5 hrs. after adding 10% HCl, III (R = R₁ = R₂ = H) is obtained, m. 130-2.degree. (Et₂O-petroleum ether). Similarly prep'd. are IIII (R = R₁ = H, R₂ = MeO), m. 119-21.degree., and III (R = H, R₁ = R₂ = MeO), m. 162-5.degree.. By treating I [R = H, R₁ = tetrahydropyranyl-2-oxy (Q)] with PhMgBr as described, but decompd. with NH₄Cl soln., II (R = R₂ = H, R₁ = Q) is obtained, while from the alk. washing fluid some II (R = R₂ = H, R₁ = OH) (VIII) is isolated. Similarly is prep'd. from IV and p-QC₆H₄MgBr II (R = R₁ = H, R₂ = Q) (IX). VII (2 g.) is refluxed 2.5 hrs. in 50 ml. 5% HCl in dil. EtOH, the mixt. cooled and extd. with CHCl₃ to yield III (R = R₂ = H, R₁ = OH) (X); similarly are obtained III (R = R₁ = H, R₂ = OH) (XI), m. 188-9.degree., from IX, and III (R = H, R₁ = MeO, R₂ = OH), m. 118.degree.. A soln. of 2 g. VI in 200 ml. EtOAc is hydrogenated at room temp. over 5% Pd-C, filtered, concd., the residue chromatographed on SiO₂, and eluted with C₆H₆ to yield II (R = R₁ = H, R₂ = OH) (XII); similarly are prep'd. II (R = H, R₁ = MeO, R₂ = OH), m.

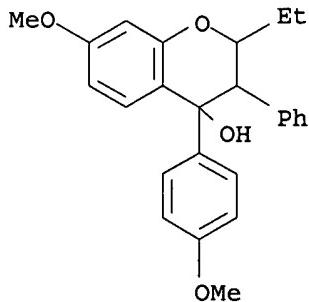
173.degree. and II (R = Et, R1 = MeO, R2 = OH), m. 112.degree. and 150-2.degree. (2 isomers). XII (0.99 g.) is heated 5 hrs. at 100.degree. with a mixt. of 0.7 ml. H₂SO₄ and 13 ml. dioxane, cooled, poured on ice, extd. with CHCl₃, the ext. concd., and the residue crystd. from Et₂O-petroleum ether to give XI, m. 188-9.degree.. X (0.5 g.) in 10 ml. Me₂CO is boiled 24 hrs. in N with 0.3 g. ClCH₂CO₂Et and 0.35 g. anhyd. K₂CO₃, concd., and extd. with CH₂Cl₂ to yield III (R = R₂ = H, R₁ = EtO₂CCH₂O) (XIII). XI (1 g.), 4 g. 2-pyrrolidinonethyl chloride, 1.2 g. dry K₂CO₃, and 40 ml. abs. Me₂CO are stirred and boiled 20 hrs., concd., the residue dild. with H₂O and Et₂O, the Et₂O layer sepd. dried, on KOH, concd., and the residue chromatographed on Al₂O₃ and eluted with CHCl₃ to give III (R = R₁ = H, R₂ = 2-pyrrolidinoethoxy), m. 98-9.degree. (Me₂CO-Et₂O). X (1 g.), 5 ml. C₅H₅N, and 5 ml. Ac₂O are heated 5 hrs. at 50.degree., cooled, and extd. with CHCl₃ to yield III (R = R₂ = H, R₁ = AcO). To a soln. of 21 ml. POCl₃ in 210 ml. abs. C₅H₅N is added with stirring in 15 min. at 5.degree. a soln. of 7.8 g. X in 105 ml. C₅H₅N; after 15 hrs. at room temp. the mixt. is poured on a mixt. of 3 kg. ice and 300 ml. concd. HCl, heated at 100.degree. for 90 min., cooled, extd. with EtOAc, the ext. washed with HCl, dried on Na₂SO₄, filtered, and concd. to yield the phosphate of X. H₂NSO₃H (6 g.) and 7.5 g. X are suspended in 5 ml. abs. C₅H₅N, stirred 90 min. at 100.degree., cooled, filtered, the filter washed with C₅H₅N, the filtrate extd. with abs. Et₂O, the residue dried in vacuo, 75 ml. 12% NaOH and 53 ml. C₅H₅N added and shaken for 5 min.; the upper C₅H₅N layer washed with Et₂O, MeOH added and concd., and the residue crystd. from MeOH to yield III (R = R₂ = H, R₁ = OSO₃Na). XIII (2 g.) is refluxed 3 hrs. with 30 ml. 2N KOH in EtOH, and the soln. acidified to yield III (R = R₂ = H, R₁ = HO₂CCH₂O); XIII (3.5 g.) is refluxed 6 hrs. in a mixt. of 2 g. pyrrolidine and 10 ml. abs. C₆H₆, and the soln. concd. to yield III (R = R₂ = H, R₁ = QCOCH₂O) (Q = pyrrolidino). II and III have antigenadotropic and contraceptive effects.

IT 13417-66-8P 13417-74-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

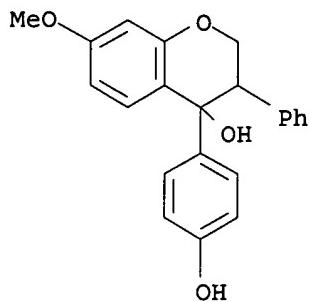
RN 13417-66-8 CAPLUS

CN 4-Chromanol, 2-ethyl-7-methoxy-4-(p-methoxyphenyl)-3-phenyl- (8CI) (CA INDEX NAME)



RN 13417-74-8 CAPLUS

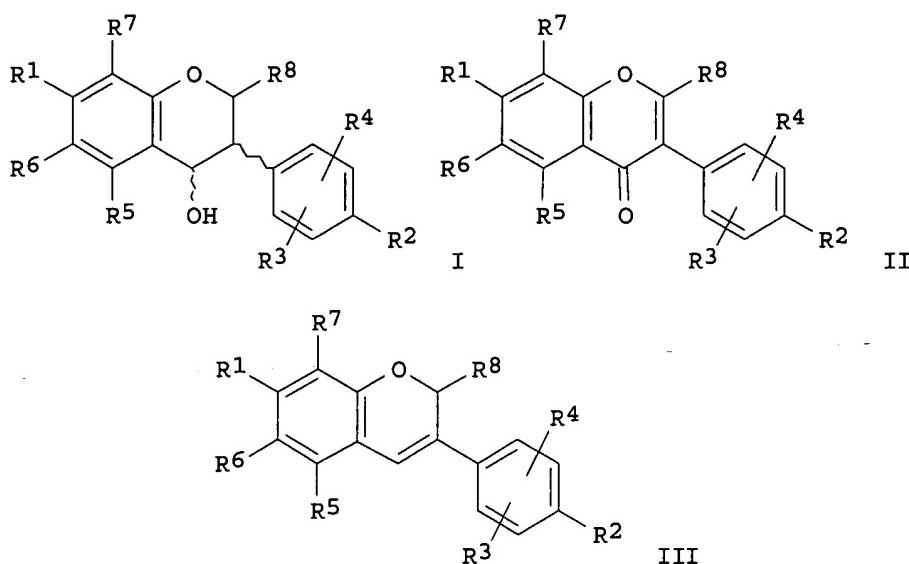
CN 4-Chromanol, 4-(p-hydroxyphenyl)-7-methoxy-3-phenyl- (8CI) (CA INDEX NAME)



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L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 2000:592710 CAPLUS
 DOCUMENT NUMBER: 133:177059
 TITLE: Preparation of isoflavone derivatives
 INVENTOR(S): Heaton, Andrew; Kumar, Naresh
 PATENT ASSIGNEE(S): Novogen Research Pty. Ltd., Australia
 SOURCE: PCT Int. Appl., 55 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--|----------|-----------------|------------|
| WO 2000049009 | A1 | 20000824 | WO 2000-AU103 | 20000215 |
| W: | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | |
| RW: | GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | |
| BR 2000008222 | A | 20011030 | BR 2000-8222 | 20000215 |
| EP 1153020 | A1 | 20011114 | EP 2000-904727 | 20000215 |
| R: | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | |
| NO 2001003945 | A | 20010814 | NO 2001-3945 | 20010814 |
| PRIORITY APPLN. INFO.: | | | AU 1999-8685 | A 19990215 |
| | | | WO 2000-AU103 | W 20000215 |
| OTHER SOURCE(S): | MARPAT 133:177059 | | | |
| GI | | | | |



AB Isoflavone derivs., such as I, II, and III [R1-8 = H, OH, SH, NH₂, NO₂, alkyl, haloalkyl, aryl, arylalkyl, alkylthio, alkylamino, dialkylamino, halo, alkyloxy, aryloxy, acyloxy, alkylsulfinyloxy, arylsulfinyloxy, etc.], were prep'd. Thus, daidzein diacetate was prep'd. in 83% yield by acetylation of daidzein with acetic anhydride in pyridine. Methods for the **hydrogenation** of isoflavones are described which provide access to workable quantities of isoflavan-4-ols, isoflavan-3-enes, and isoflavans. The isoflavone derivs. can be obtained in high purity and in near quant. yields while employing pharmaceutically acceptable reagents and solvents.

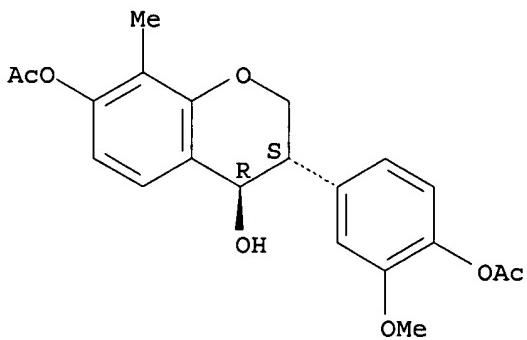
IT 288266-89-7P

RL: RCT (Reactant); SPN (Synthetic preparation); **PREP** (**Preparation**); RACT (Reactant or reagent)
(prep'n. of isoflavone derivs.)

RN 288266-89-7 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3-[4-(acetyloxy)-3-methoxyphenyl]-3,4-dihydro-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 288266-88-6P

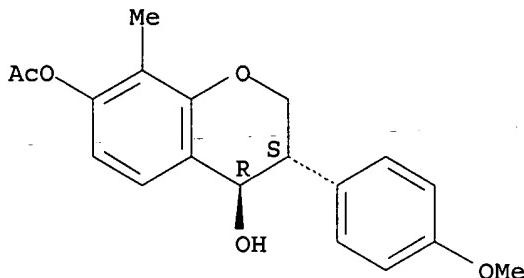
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prep. of isoflavone derivs.)

RN 288266-88-6 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-(4-methoxyphenyl)-8-methyl-, 7-acetate, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



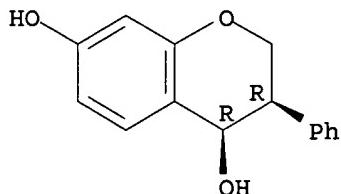
IT 288267-21-0P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prep. of isoflavone derivs.)

RN 288267-21-0 CAPLUS

CN 2H-1-Benzopyran-4,7-diol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1986:148589 CAPLUS

DOCUMENT NUMBER: 104:148589

TITLE: The chemistry of the 'insoluble red woods'. Part 16.
 Some further observations on the condensation of

isoflavylium salts with 1,3-diphenylpropenes

Afonya, Theophilus C. A.; Epelle, Faithwin B. M.;
 Osman, Soad A. A.; Whalley, W. Basil

CORPORATE SOURCE: Sch. Pharm., London, WC1N 1AX, UK

SOURCE: J. Chem. Res., Synop. (1985), (10), 305

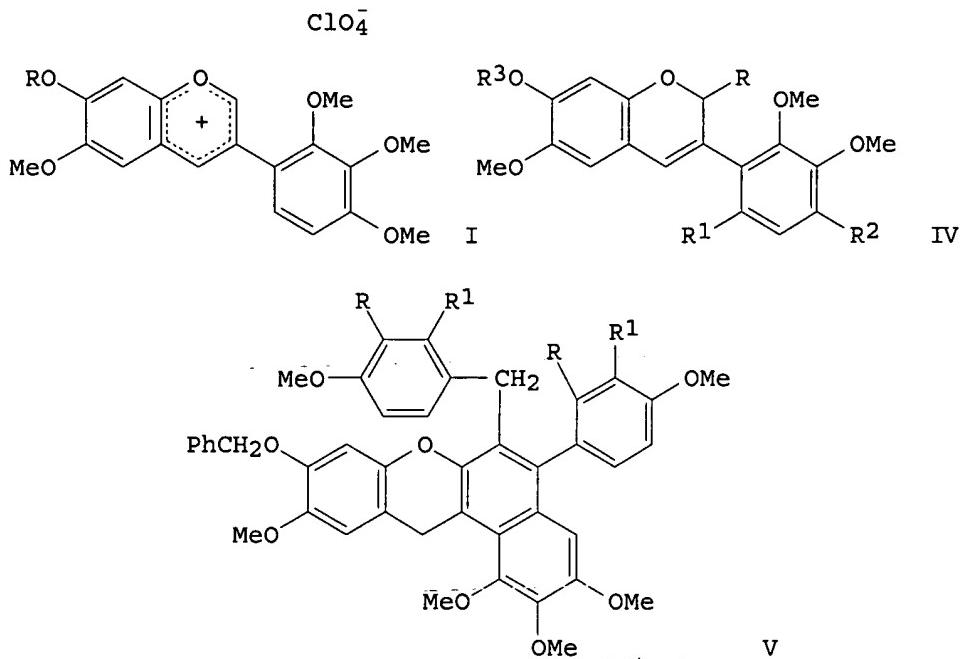
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:148589

GI



AB Condensation of isoflavylium perchlorate I ($R = \text{CH}_2\text{Ph}$) (II) with $3,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{CH}:\text{CHCH}_2\text{C}_6\text{H}_3(\text{OMe})_2-2,4$ (III) in refluxing MeCN for 3 h gave isoflavene IV ($R = R_1 = \text{H}$, $R_2 = \text{OMe}$, $R_3 = \text{CH}_2\text{Ph}$) and benzoxanthene V ($R = \text{H}$, $R_1 = \text{OMe}$). Similar reaction of II with $2,4-(\text{MeO})_2\text{C}_6\text{H}_3\text{CH}:\text{CHCH}_2\text{C}_6\text{H}_3(\text{OMe})_2-3,4$ (VI) gave isoflavene IV ($R = R_2 = \text{OMe}$, $R_1 = \text{H}$; $R = R_2 = \text{H}$, $R_1 = \text{OMe}$; $R_3 = \text{CH}_2\text{Ph}$) and benzoxanthene V ($R = \text{OMe}$, $R_1 = \text{H}$). Analogous reaction of I ($R = \text{Me}$) with III or VI gave only the isoflavene IV ($R = R_2 = \text{OMe}$, $R_1 = \text{H}$, $R_3 = \text{Me}$). The preps. of the starting materials are reported.

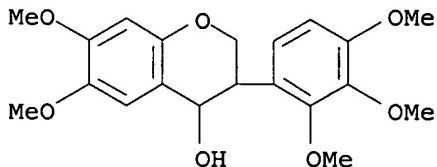
IT 100753-48-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation)

(prepn. and elimination reaction of, isoflavylium salt by)

RN 100753-48-8 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-6,7-dimethoxy-3-(2,3,4-trimethoxyphenyl)-
(9CI) (CA INDEX NAME)



=> log y
COST IN U.S. DOLLARS
FULL ESTIMATED COST

| | |
|------------|---------|
| SINCE FILE | TOTAL |
| ENTRY | SESSION |
| 47.95 | 49.32 |

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FILE COVERS 1907 - 19 Sep 2002 VOL 137 ISS 12
FILE LAST UPDATED: 18 Sep 2002 (20020918/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> d his

(FILE 'HOME' ENTERED AT 09:21:28 ON 19 SEP 2002)

FILE 'REGISTRY' ENTERED AT 09:24:47 ON 19 SEP 2002

L1 STRUCTURE UPLOADED
L2 0 S L1
L3 28 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 09:25:53 ON 19 SEP 2002

=> s l3
L4 23 L3

=> s l3/proc
 23 L3
 3207019 PROC/RL
L5 1 L3/PROC

 (L3 (L) PROC/RL)

=> s l3 and hydrogenation?

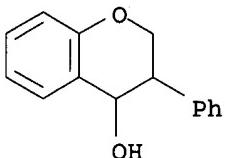
 23 L3
 150237 HYDROGENATION?
L6 4 L3 AND HYDROGENATION?

=> d ibib abs hitstr 14 tot

L4 ANSWER 1 OF 23 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:596845 CAPLUS
DOCUMENT NUMBER: 131:233400
TITLE: Tyrosinase inhibitors containing flavonoids and cosmetics containing the inhibitors
INVENTOR(S): Sakai, Katsuki; Kondo, Ryuichiro; Shimizu, Kuniyoshi; Sato, Hiroaki
PATENT ASSIGNEE(S): Kansai Koso K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

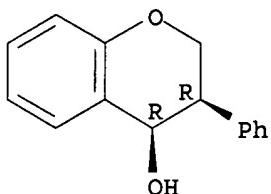
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|----------|-----------------|----------|
| JP 11255637 | A2 | 19990921 | JP 1998-63167 | 19980313 |
| OTHER SOURCE(S) : MARPAT 131:233400 | | | | |
| AB Tyrosinase inhibitors contain .gtoreq.1 agent selected from the group consisting of resorcinol derivs. and hydroxy flavonoids as active ingredients. Cosmetics contg. the tyrosinase inhibitors are also claimed. Anthocyanin extd. from natural products was gradually added dropwise to HNO ₃ /H ₂ SO ₄ at 0.degree. and the reaction mixt. was further stirred at room temp. for 3 h to give 2',4'-dinitroanthocyanin. This was reduced and the resulting 2',4'-diaminoanthocyanin was further treated with HNO ₂ /HCl to give 2',4'-dihydroxyanthocyanin. IC ₅₀ of the compd. against tyrosinase was 2.8 .mu.M. A cream contg. 2',4'-dihydroxyaurone was also formulated. | | | | |
| IT 1481-96-5 | RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of hydroxy flavonoids as tyrosinase inhibitors for skin-lightening cosmetics) | | | |
| RN 1481-96-5 CAPLUS | | | | |
| CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) | (CA INDEX NAME) | | | |



L4 ANSWER 2 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1999:503614 CAPLUS
 DOCUMENT NUMBER: 131:266558
 TITLE: Binding affinity to steroid hormone receptors and antiproliferative action on MCF-7 cells of coumarinic derivatives and isoflavonoids
 AUTHOR(S): Kirkiacharian, S.; Chidiack, H.; Philibert, D.; Van De Velde, P.; Bouchoux, F.
 CORPORATE SOURCE: Lab. Chim. Therapeutique, Fac. Pharmacie de Paris-Sud, Jean-Baptiste-Clement, Chatenay-Malabry, F 92296, Fr.
 SOURCE: Annales Pharmaceutiques Francaises (1999), 57(4), 332-339
 CODEN: APFRAD; ISSN: 0003-4509
 PUBLISHER: Masson Editeur
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 AB The study of the relative binding affinity to steroid hormonal receptors and of the antiproliferative action on MCF-7 cells of 3-arylcoumarines, 3-aryl-4-hydroxycoumarines, isoflavanones, isoflavan-4-ols and isoflavones, indicates a weak activity in the case of some representatives of coumarines.
 IT 6212-70-0 20986-77-0
 RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
 (binding affinity to steroid hormone receptors and antiproliferative action on MCF-7 cells of coumarin derivs. and isoflavonoids)
 RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX
NAME)

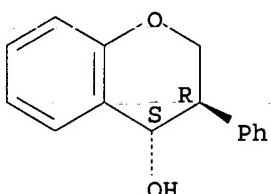
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX
NAME)

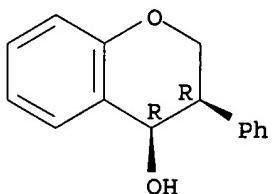
Relative stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1998:256815 CAPLUS
 DOCUMENT NUMBER: 129:54205
 TITLE: Diastereoselectivity of various routes to isoflavan-4-ols (3-phenyl-4-chromanols)
 AUTHOR(S): Chidiak, Henry; Kirkiacharyan, S.
 CORPORATE SOURCE: Lab. Chim. Ther. Fac. Pharm., Univ. Paris, Paris, Fr.
 SOURCE: Khimicheskii Zhurnal Armenii (1996), 49(1-3), 94-104
 CODEN: KZARF3
 PUBLISHER: Izdatel'stvo Gitutyun NAN Respubliki Armenii
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The redn. of isoflavan-4-ones (3-phenyl-4-chromanones) by nucleophilic hydrides (sodium borohydride, lithium aluminum tri-tert-butoxyhydride, lithium tri-sec-butylborohydride) leads to mixts. of cis and trans diastereoisomers of isoflavan-4-ols. Redn. by electrophilic hydrides (borane-THF, bis-tert-butylthioethane diborane, or 9-borabicyclo[3.3.1]nonane) is stereoselective and forms cis diastereoisomers in excellent yields. Hydroboration, followed by alk. hydroperoxide oxidn., of 3-phenyl-4-hydroxycoumarins is a stereoselective route to trans diastereoisomers of isoflavan-4-ols.
 IT 6212-70-0P, 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, cis-
 20986-77-0P, 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, trans-
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (diastereoselectivity of various routes to isoflavan-4-ols)
 RN 6212-70-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX
NAME)

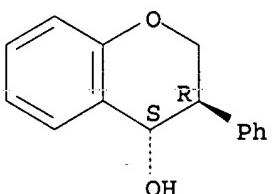
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 4 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1990:631155 CAPLUS

DOCUMENT NUMBER: 113:231155

TITLE: Structure-activity relationship of antiestrogens.
Effect of the side chain and its position on activity
of 2,3-diaryl-2H-1-benzopyrans

AUTHOR(S): Sharma, Arun P.; Saeed, Ashraf; Durani, Susheel;
Kapil, Randhir S.

CORPORATE SOURCE: Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226
001, India

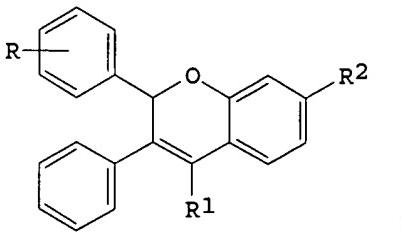
SOURCE: J. Med. Chem. (1990), 33(12), 3216-22
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:231155

GI



AB A series of diarylbenzopyrans (I; R = tertiary aminoethoxy, in ortho,
meta, or para position, R1 = H, Me, Et; R2 = H, OMe;) were synthesized and
evaluated for their affinity for estrogen receptor (ER), for microsomal

antiestrogen specific binding site and for their uterotrophic-antiuterotrophic activities in rodents. The analogs bearing the side chain at the para position of 2-Ph were found to be active while those substituted at the meta and ortho positions were inactive as ER ligands as well as estrogen agonists-antagonists. Among para-substituted ethers, analog [I; R = (2-piperidinyl)ethoxy (II)] was found to be a more effective antiestrogen, than the corresponding pyrrolidinyl, dimethylamino, and related analogs. Incorporation of Me or Et at C4 in the pyran nucleus was found to increase receptor affinity of the prototypes. The Et was also found to potentiate agonist activity of the prototype, while abolishing its antagonist activity. Analog (II) was found to be a better antiestrogen than tamoxifen as well as LY-117018 in rats as well as mice. The prototypes were also found to have high affinity for the microsomal antiestrogen specific binding sites. The benzopyrans have thus emerged as a new group of potent antiestrogens.

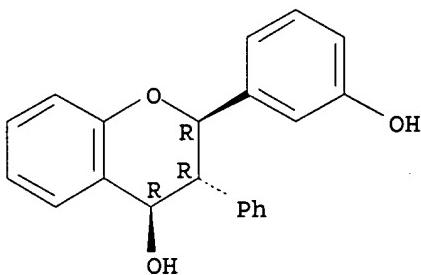
IT 130406-81-4P 130406-82-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepns. and dehydration of)

RN 130406-81-4 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-2-(3-hydroxyphenyl)-3-phenyl-,
(2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

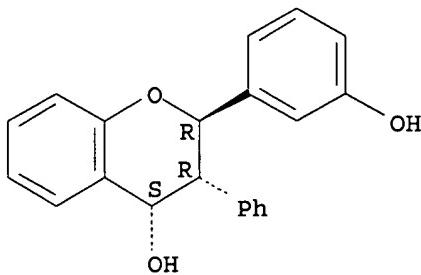
Relative stereochemistry.



RN 130406-82-5 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-2-(3-hydroxyphenyl)-3-phenyl-,
(2.alpha.,3.beta.,4.beta.)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 5 OF 23 CAPLUS COPYRIGHT 2002 ACS

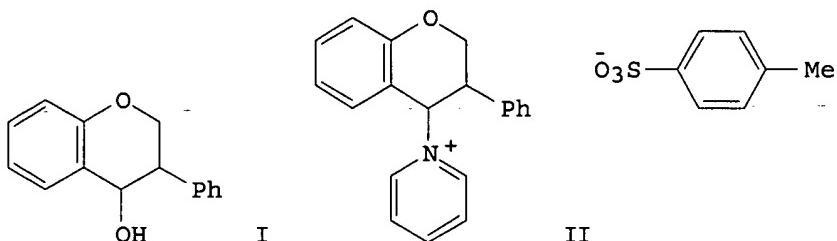
ACCESSION NUMBER: 1980:215213 CAPLUS

DOCUMENT NUMBER: 92:215213

TITLE: Syntheses of isoflavan-4-(1-pyridinium) salts

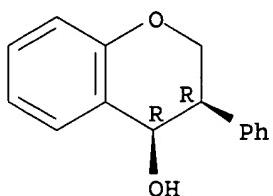
AUTHOR(S): Szabo, Vince; Borbely, Janos; Antal, Erno

CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Lajos Univ., Debrecen,
H-4010, Hung.
 SOURCE: Acta Chim. Acad. Sci. Hung. (1979), 102(1), 51-7
 CODEN: ACASA2; ISSN: 0001-5407
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



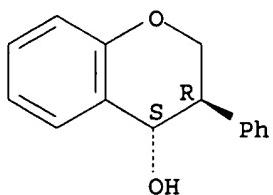
- AB Treatment of trans(.alpha.)- or cis(.beta.)-4-hydroxyisoflavan (I) with p-MeC₆H₄SO₂Cl in pyridine gives, instead of the expected tosylates, the same isoflavan-4-(1-pyridinium) tosylate (II). The anion of II is exchangeable for other anions. Reductive methods convert II to isoflavin and 4-[1-(1,4-dihydropyridyl)]isoflavan; in alk. medium it can be converted to isoflav-3-ene.
- IT 6212-70-0P 20986-77-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (prepn. and reaction with toluenesulfonyl chloride and pyridine)
- RN 6212-70-0 CAPLUS
- CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

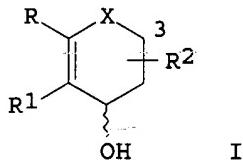


- RN 20986-77-0 CAPLUS
- CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 6 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1979:507355 CAPLUS
 DOCUMENT NUMBER: 91:107355
 TITLE: A hydroxyl proton magnetic resonance study of
 2-cyclohexen-1-ols, 1-tetralols, 4-chromanols, and
 4-thiochromanols in dimethyl sulfoxide
 AUTHOR(S): Hanaya, Kaoru; Kudo, Hideaki; Gohke, Kazuo; Imaizumi,
 Shin
 CORPORATE SOURCE: Fac. Sci., Yamagata Univ., Yamatata, 990, Japan
 SOURCE: Bull. Chem. Soc. Jpn. (1979), 52(7), 2163-4
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB The ^1H NMR spectra of title epimeric alcs. I ($\text{X} = \text{CH}_2$, $\text{R} = \text{H}$, $\text{R}1 = \text{Me}$, $\text{R}2 = 3\text{-Me}_3\text{C}$ or $\text{R}1 = \text{H}$, $\text{R}2 = 3\text{-Ph}$; $\text{X} = \text{CH}_2$, O , S , SO_2 ; $\text{R}1 = \text{benzo}$, $\text{R}2 = 2\text{- or}$
 3-Me or -Ph) showed that in all cases the pseudoaxial OH proton resonates
 at a higher field than the pseudoequatorial proton. The spin-spin
 coupling between the OH and carbonyl protons is greater for the
 pseudoequatorial epimer than for the pseudoaxial epimer.

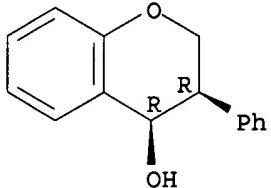
IT 6212-70-0 20986-77-0

RL: PRP (Properties)
 (NMR spectrum of)

RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX
 NAME)

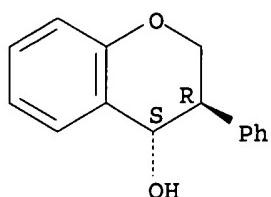
Relative stereochemistry.



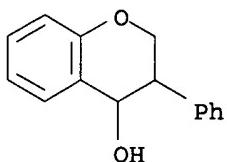
RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX
 NAME)

Relative stereochemistry.



L4 ANSWER 7 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1977:120467 CAPLUS
 DOCUMENT NUMBER: 86:120467
 TITLE: Reductive conversions of chromanoids. I. Catalytic hydrogenation of isoflavone (3-phenylchromone)
 AUTHOR(S): Szabo, Vince; Antal, Erno
 CORPORATE SOURCE: Dep. Appl. Chem., Kossuth Lajos Univ., Debrecen, Hung.
 SOURCE: Acta Chim. Acad. Sci. Hung. (1976), 90(4), 381-93
 CODEN: ACASA2
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A kinetic study of the hydrogenation of isoflavone over a Pd/C catalyst showed that the rate and the product distribution are dependent upon the solvent, pH of the soln., and the activity of the catalyst. Selective hydrogenation, by appropriate choice of conditions, gave predominantly isoflavanone, 4-isoflavanol, isoflavan, or, in dil. alkali, 2-hydroxy-.alpha.-methyldeoxybenzoin.
 IT 1481-96-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 1481-96-5 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



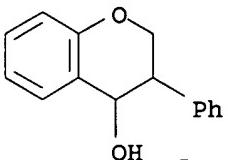
L4 ANSWER 8 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1976:542925 CAPLUS
 DOCUMENT NUMBER: 85:142925
 TITLE: The reactivity of 4-hydroxyisoflavan. Synthesis of 4-(1-pyridinium)isoflavans
 AUTHOR(S): Szabo, V.; Antal, E.
 CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Lajos Univ., Debrecen, Hung.
 SOURCE: Top. Flavonoid Chem. Biochem., Proc. Hung. Bioflavonoid Symp., 4th (1975), Meeting Date 1973, 139-43. Editor(s): Farkas, L.; Gabor, M.; Kallay, F. Elsevier: Amsterdam, Neth.
 CODEN: 32YSAR
 DOCUMENT TYPE: Conference; General Review
 LANGUAGE: English
 AB A review with no refs.

IT 1481-96-5

RL: PRP (Properties)
(reactivity of)

RN 1481-96-5 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 9 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:593003 CAPLUS

DOCUMENT NUMBER: 83:193003

TITLE: Oxidation of 2'-hydroxy-.alpha.-phenylchalcones.
Substiuient effects on the course of the
Algar-Flynn-Oyamada (AFO) reactionAUTHOR(S): Cullen, William P.; Donnelly, Derville M. X.; Keenan,
Alan K.; Kennan, Patrick J.; Ramdas, K.

CORPORATE SOURCE: Dep. Chem., Univ. Coll., Dublin, Ire.

SOURCE: J. Chem. Soc., Perkin Trans. 1 (1975), (17), 1671-4
CODEN: JCPRB4

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB E-2,4,6-(HO)R₂C₆H₂COCPH:CHPh (I; R = H, MeO) in alk. H₂O₂ gave the chromanone II. The cyclization at the .beta.-position occurred due to coulombic repulsion of the .alpha.-Ph group by the PhO-. 2,1-(HO)(PhCH:CPHCO)C₁₀H₆ on AFO oxidn. gave a 1:1 mixt. of the .beta.- (III) and .alpha.-cyclization (IV) products.

IT 57642-73-6P 57642-76-9P 57642-78-1P

57642-79-2P 57642-80-5P 57642-81-6P

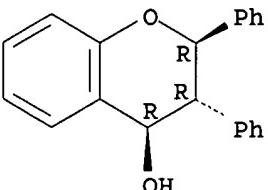
57642-83-8P 57642-84-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

RN 57642-73-6 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-2,3-diphenyl-,
(2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

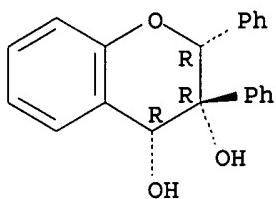
Relative stereochemistry.



RN 57642-76-9 CAPLUS

CN 2H-1-Benzopyran-3,4-diol, 3,4-dihydro-2,3-diphenyl-,
(2.alpha.,3.alpha.,4.alpha.)- (9CI) (CA INDEX NAME)

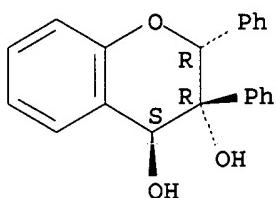
Relative stereochemistry.



RN 57642-78-1 CAPLUS

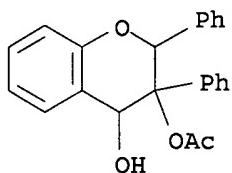
CN 2H-1-Benzopyran-3,4-diol, 3,4-dihydro-2,3-diphenyl-,
(2. α .,3. α .,4. β .)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 57642-79-2 CAPLUS

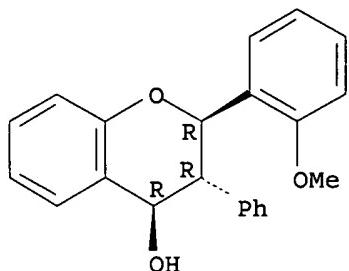
CN 2H-1-Benzopyran-3,4-diol, 3,4-dihydro-2,3-diphenyl-, 3-acetate,
(2. α .,3. α .,4. β .)- (9CI) (CA INDEX NAME)



RN 57642-80-5 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-2-(2-methoxyphenyl)-3-phenyl-,
(2. α .,3. β .,4. α .)- (9CI) (CA INDEX NAME)

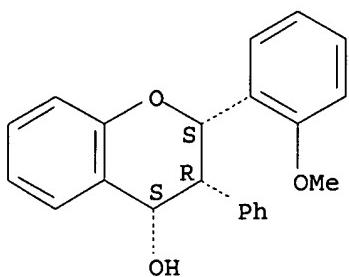
Relative stereochemistry.



RN 57642-81-6 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-2-(2-methoxyphenyl)-3-phenyl-,
(2. α .,3. α .,4. α .)- (9CI) (CA INDEX NAME)

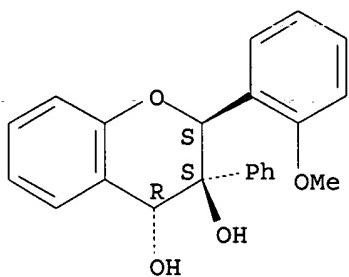
Relative stereochemistry.



RN 57642-83-8 CAPLUS

CN 2H-1-Benzopyran-3,4-diol, 3,4-dihydro-2-(2-methoxyphenyl)-3-phenyl-, (2. α .,3. α .,4. β .)- (9CI) (CA INDEX NAME)

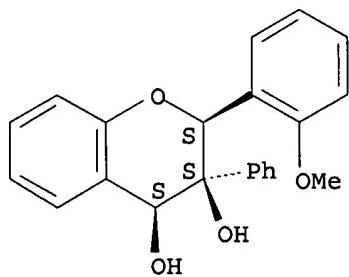
Relative stereochemistry.



RN 57642-84-9 CAPLUS

CN 2H-1-Benzopyran-3,4-diol, 3,4-dihydro-2-(2-methoxyphenyl)-3-phenyl-, (2. α .,3. α .,4. α .)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 10 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1973:504410 CAPLUS

DOCUMENT NUMBER: 79:104410

TITLE: Mass spectral study of phenyltetralols and phenylchromanols

AUTHOR(S): Sasaki, Shinichi; Abe, Hidetsugu; Suzuki, Minoru; Sakuraba, Yukio; Ohtomo, Miki

CORPORATE SOURCE: Miyagi Univ. Educ., Sendai, Japan

SOURCE: Shitsuryo Bunseki (1973), 21(2), 195-8

CODEN: SHIBAK

DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB The mass spectra of 16 compds. belonging to phenyltetralols and phenylchromanols were measured. The fragmentation pathways and the behavior of water elimination of these compds. upon electron impact were described.

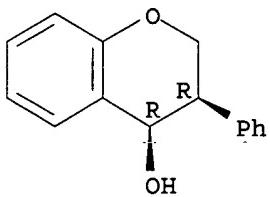
IT 6212-70-0 20986-77-0

RL: PRP (Properties)
(mass spectrum of)

RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

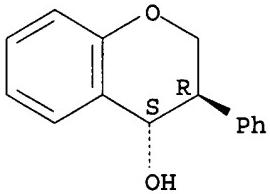
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



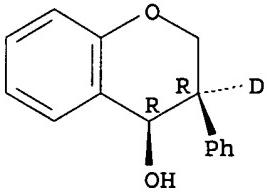
IT 42288-90-4P 42288-91-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 42288-90-4 CAPLUS

CN 2H-1-Benzopyran-3-d-4-ol, 3,4-dihydro-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

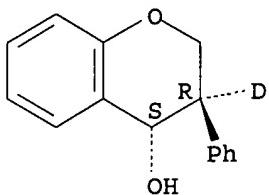


RN 42288-91-5 CAPLUS

CN 2H-1-Benzopyran-3-d-4-ol, 3,4-dihydro-3-phenyl-, trans- (9CI) (CA INDEX

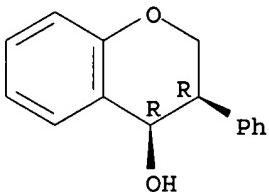
NAME)

Relative stereochemistry.



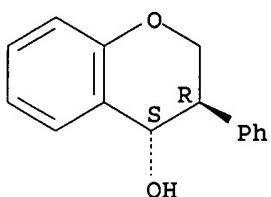
L4 ANSWER 11 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1973:491915 CAPLUS
 DOCUMENT NUMBER: 79:91915
 TITLE: Selective reduction of isoflavone
 AUTHOR(S): Szabo, Vince; Antal, Erno
 CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Univ., Debrecen, Hung.
 SOURCE: Tetrahedron Lett. (1973), (19), 1659-62
 CODEN: TELEAY
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Isoflavone (I) with Pd-H in EtOH or dioxane gave isoflavan-4-ol (II, R = H,OH) and isoflavanone (II, R = O), resp., almost quant. The effect of pH on the hydrogenation of I in buffered aq. EtOH was studied and thereby 90% II (R = O) was obtained by stopping the reaction after the absorption of 1 mole of H. At pH .gtoreq.11.5 2-HOC₆H₄COCHRPh (R = H and Me) was formed.
 IT 6212-70-0P 20986-77-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 6212-70-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



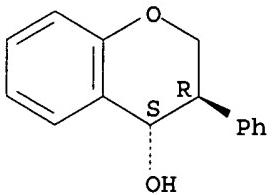
RN 20986-77-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 12 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1973:159372 CAPLUS
 DOCUMENT NUMBER: 78:159372
 TITLE: New synthesis of isoflavanol, isoflavanone, and isoflavone
 AUTHOR(S): Kirkiacharian, Berdj Serge; Chidiack, Henri
 CORPORATE SOURCE: Lab. Pharm. Chem., Fac. Fr. Med. Pharm., Beirut, Lebanon
 SOURCE: C. R. Acad. Sci., Ser. C (1973), 276(9), 795-8
 CODEN: CHDDAT
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB The 4-hydroxy-3-phenylchromans I (R=H, Me, OMe) were obtained by NaBH4 redn. of the coumarins II. Cr2O3 oxidn. of I (R=H) gave isoflavanone, which was dehydrogenated to isoflavone by heating with Pd-C.
 IT 20986-77-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 RN 20986-77-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 13 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1972:564397 CAPLUS
 DOCUMENT NUMBER: 77:164397
 TITLE: New synthesis of trans-isoflavan-4-ol
 AUTHOR(S): Arai, Mannosuke; Kabuto, Kuninobu; Horino, Hiroshi; Inoue, Naoto
 CORPORATE SOURCE: Coll. Gen. Educ., Tohoku Univ., Sendai, Japan
 SOURCE: Chem. Lett. (1972), (10), 889-90
 CODEN: CMLTAG
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The title compd. was prep'd. in 61 yield by treating chromene with Li2PdCl4 and PhHgCl in aq. Me2CO. Cis-Isoflavan-4-ol and isoflavene were also formed in the reaction.

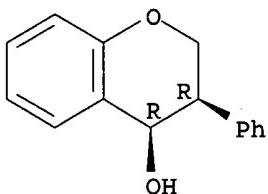
IT 6212-70-0P 20986-77-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX
NAME)

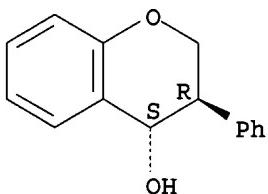
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX
NAME)

Relative stereochemistry.



L4 ANSWER 14 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1972:126247 CAPLUS

DOCUMENT NUMBER: 76:126247

TITLE: Oxidation of chroman-4-ols with chromic acid

AUTHOR(S): Yamaguchi, Shozo; Kabuto, Kuninobu; Kikuchi, Yoriko;
Inoue, Naoto

CORPORATE SOURCE: Coll. Gen. Educ., Tohoku Univ., Sendai, Japan

SOURCE: Bull. Chem. Soc. Jap. (1971), 44(12), 3487

CODEN: BCSJA8

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rate of oxidn. of chroman-4-ols with chromic acid and their isotope effect were detd. Chromanols contg. a cis-2-substituent had the fastest rate owing to stereoelectronic effects and the relief of A strain. The oxidn. of 3-substituted chromanols was also discussed.

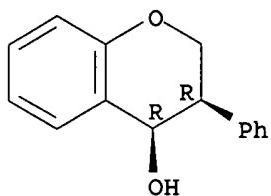
IT 6212-70-0 20986-77-0

RL: RCT (Reactant)
(oxidn. of, kinetics of)

RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX
NAME)

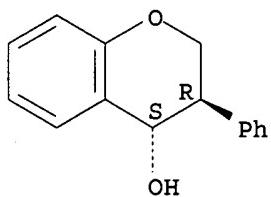
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 15 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:476524 CAPLUS

DOCUMENT NUMBER: 75:76524

TITLE: Reactions of isoflavanones with Grignard reagents.
Synthesis of estrogenic and antiestrogenic active
isoflavanoids

AUTHOR(S): Irmischer, Klaus; Borck, Joachim

CORPORATE SOURCE: Chem. Forsch. E. Merck, Darmstadt, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1971), 744, 164-77

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

GI For diagram(s), see printed CA Issue.

AB Grignard reaction of isoflavanones or 2-ethyl-7-methoxyisoflavanones (I) gave 4-aryl-4-isoflavanols or 2-ethyl-7-methoxy-4-aryl-4-isoflavanols (II), resp., which were dehydrated to 4-aryl-3-isoflavenes. Depending on the reaction conditions, the constitution of the isoflavanone, and the Grignard reagent, the C-2 atom of the isoflavanone was also attached in some cases to give .beta.-aryl-.alpha.-phenyl-2-hydroxypropiophenones with ring opening. The mechanism of the ring opening involving an .alpha.-methylene ketone was discussed.

IT 33103-09-2P 33103-10-5P 33103-11-6P

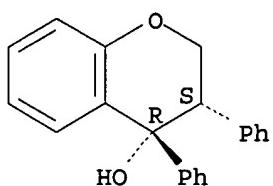
33103-12-7P 33279-52-6P 33279-53-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

RN 33103-09-2 CAPLUS

CN 4-Chromanol, 3,4-diphenyl-, stereoisomer (8CI) (CA INDEX NAME)

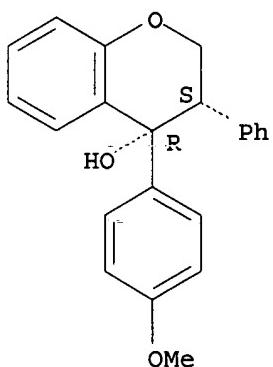
Relative stereochemistry.



RN 33103-10-5 CAPLUS

CN 4-Chromanol, 4-(p-methoxyphenyl)-3-phenyl-, stereoisomer (8CI) (CA INDEX NAME)

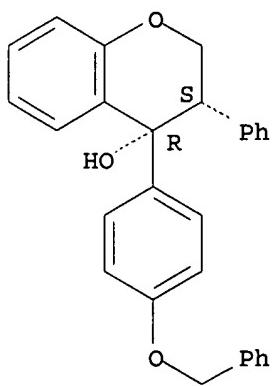
Relative stereochemistry.



RN 33103-11-6 CAPLUS

CN 4-Chromanol, 4-[p-(benzyloxy)phenyl]-3-phenyl-, stereoisomer (8CI) (CA INDEX NAME)

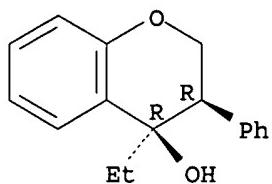
Relative stereochemistry.



RN 33103-12-7 CAPLUS

CN 4-Isoflavanol, 4-ethyl-, stereoisomer (8CI) (CA INDEX NAME)

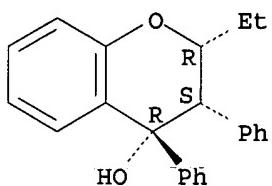
Relative stereochemistry.



RN 33279-52-6 CAPLUS

CN 4-Chromanol, 2-ethyl-3,4-diphenyl-, stereoisomer (8CI) (CA INDEX NAME)

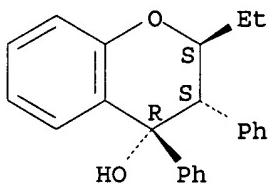
Relative stereochemistry.



RN 33279-53-7 CAPLUS

CN 4-Chromanol, 2-ethyl-3,4-diphenyl-, stereoisomer (8CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 16 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1971:87232 CAPLUS

DOCUMENT NUMBER: 74:87232

TITLE: Conformation of trans-4-acetoxyisoflavans and related compounds

AUTHOR(S): Yamaguchi, Shozo; Kabuto, Kuninobu; Ninomiya, Yoriko; Inoue, Naoto

CORPORATE SOURCE: Coll. Gen. Educ., Tohoku Univ., Sendai, Japan

SOURCE: Bull. Chem. Soc. Jap. (1970), 43(12), 3952-4

CODEN: BCSJA8

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The isoflavans and chromans I-VI exist preferentially in the conformation with the substituent in the 4-position in a quasi-axial environment. The conformation in I-III is attributed to A(1,3)-strain (pseudo allylic effect) of the conformations having equatorial substituents. The hydroxy-isoflavans corresponding to I-III (R₂ = H) and VII exist in the equatorial conformations having equatorial substituents because the A(1,3)-strain is partially overcome by intramol. H-bonding of the C-3 phenyl groups with the OH group. VI is apprx.81 in the conformation in

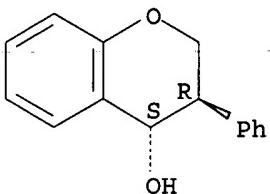
which the substituents are axial and has an allylic strain of 1.1-1.2 kcal/mole.

IT 20986-77-0
 RL: PRP (Properties)
 (conformation of)

RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 17 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1971:52906 CAPLUS
 DOCUMENT NUMBER: 74:52906
 TITLE: .nu. O-H absorptions and conformations of epimeric 1-tetralols and chroman-4-ols

AUTHOR(S): Iwamura, Hiizu; Hanaya, Kaoru
 CORPORATE SOURCE: Fac. Sci., Univ. Tokyo, Tokyo, Japan
 SOURCE: Bull. Chem. Soc. Jap. (1970), 43(12), 3901-8
 CODEN: BCSJA8

DOCUMENT TYPE: Journal
 LANGUAGE: English

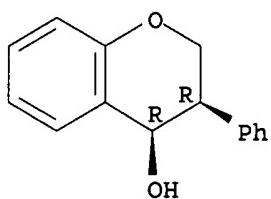
AB The O-H stretching ir absorptions of epimeric 1-tetralols and chroman-4-ols were examd. in dil. CC14 solns. The absorption pattern was related to the conformation of the OH group; the epimers with the quasi-axial OH group showed a singlet vO-H at 3618 cm⁻¹, while those with the quasiequatorial hydroxyl had doublet absorption at 3622 and 3600 cm⁻¹. Based on these findings 1-tetralol was shown to exist preferentially in the OH axial conformation. The bands at 3618 and 3600 cm⁻¹ were assigned severally to the OH groups bonding to the .pi.-electrons on the benzene ring. When an addnl. aryl group is present .beta. to the hydroryl, another O-H....pi. bonding to the aryl group becomes possible in addn. to that between the OH group and the benzene ring of the Tetralin and the chroman skeletons. The conformation of the aryl substituents was deduced by applying the empirical correlation relating the geometry of the mol. to the bonded vO-H frequency in a wide variety of aromatic alcs. which incorporate .beta.-arylethanol moiety.

IT 6212-70-0 20986-77-0
 RL: PRP (Properties)
 (conformation of, ir spectrum in relation to)

RN 6212-70-0 CAPLUS

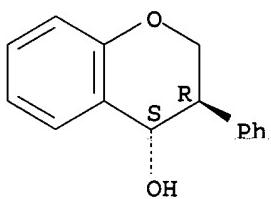
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



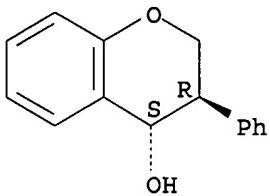
RN 20986-77-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 18 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1969:11493 CAPLUS
 DOCUMENT NUMBER: 70:11493
 TITLE: Syntheses of trans-isoflavan-4-ols
 AUTHOR(S): Yamaguchi, Shozo; Ito, Shoei; Suzuki, Ikuko; Inoue, Naoto
 CORPORATE SOURCE: Tohoku Univ., Sendai, Japan
 SOURCE: Bull. Chem. Soc. Jap. (1968), 41(9), 2073-7
 CODEN: BCSJA8
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB The reaction of nitrous acid and three 4-aminoisoflavan hydrochlorides (I, II, and III) obtained by the catalytic hydrogenation of isoflavanone oximes, and the hydroboration of 3 isoflavenes (IV, V, and VI), were investigated in the hope of finding a general method of synthesizing trans-isoflavan-4-ols. The reaction of I and II with nitrous acid afforded the corresponding trans-4-ols, though in a poor yield, but that of III produced no expected compd., the corresponding isoflavene VI being obtained instead. The hydroboration of IV, V, and VI afforded the corresponding trans-alcs. (VII, VIII, and IX) in good yields. In addn., it became clear that 4-aminoisoflavans obtained by the catalytic redn. of the oximino compds. possess the 3,4-cis configuration.
 IT 20986-77-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 RN 20986-77-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 19 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1968:39474 CAPLUS
 DOCUMENT NUMBER: 68:39474
 TITLE: 4-[p-(2-Aminoethoxy)phenyl]-3-phenylchromans
 INVENTOR(S): Carney, Richard W. J.; Bencze, William L.
 PATENT ASSIGNEE(S): CIBA Corp.
 SOURCE: U.S., 10 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|----------|
| US 3340276 | | 19670905 | US | 19640401 |

GI For diagram(s), see printed CA Issue.
 AB Compds. of the general formula I are prep'd. and can be used as estrogenic and antifertility agents. A mixt. of 100 g. PhOH and 169 g. PhCH₂COCl (sic) is refluxed 1 hr. to give 223 g. BzOPh, m. 39-41.degree.. Similarly prep'd. is m-MeOC₆H₄OBz (II), m. 85-7.degree. (EtOH). A mixt. of 223 g. BzOPh and 160 g. AlCl₃ is heated 30 min. at 170.degree. to give 42.4 g. 0-HOC₆H₄COPh (III), m. 53-4.degree. (ligroine-Et₂O). A mixt. of 10 g. III, 125 ml. pyridine, 5 ml. piperidine, and 95 ml. HC(OEt)₃ is refluxed 8 hrs. to give 6.2 g. 3-phenyl-4H-chromen-4-one (IV), m. 131-3.degree. (EtOH). A mixt. of 17.6 g. IV, 9.1 g. NaBH₄, and 800 ml. EtOH is refluxed 1 hr. to give 15.8 g. 3-phenylchroman-4-ol (V), b₁ 130-60.degree.. A soln. of 14.8 g. of V and 5.7 g. PhOH in 78 ml. hexane and 78 ml. C₆H₆ is slowly added to a cooled mixt. of 4.4 g. AlCl₃ and 12.2 g. PhOH; the mixt. is agitated overnight at room temp. to give 16 g. 4-(p-hydroxyphenyl)-3-phenylchroman (VI), b₂ 120-45.degree., m. 63.degree.. Similarly prep'd. is 4-(p-hydroxyphenyl)-7-methoxy-3-phenylchroman, m. 184.degree. (C₆H₆). A soln. of VI in 15 ml. HCONMe₂ and 15 ml. PhMe is cooled and treated with 0.2 g. 53% Na suspension, 0.84 g. Et₂NCH₂CH₂Cl in 5 ml. PhMe is added, and the mixt. is agitated overnight to give 1.5 g. 4-[p-(2-diethyloaminoethoxy)phenyl]-3-phenylchroman, b₁ 123-30.degree.. Similarly prep'd. are the following I (NR₂ = pyrrolidinyl) (X and b.p./mm. given): H, 140-50.degree./0.6; MeO, 120-40.degree./3. A mixt. of 86 g. II, 1000 ml. Et₂O, 112 g. KCN, and 500 ml. water is agitated and 200 ml. 30% H₂SO₄ is slowly added to give 93 g. Ph(m-MeOC₆H₄O)CHCH(OH)CN (VII), m. 86-7.degree.. A soln. of 23 g. VII in 400 ml. Et₂O is treated with 12 g. ZnCl₂, HCl gas is introduced into the mixt. for 2 hrs., and the mixt. is cooled 3 days to give 8.3 g. 3-hydroxy-7-methoxy-3-phenylchroman-4-one (VIII), m. 133-5.degree. (EtOAc). A mixt. of 8.3 g. VIII, 25 ml. pyridine, 25 ml. Ac₂O is heated 3 hrs. at 100-15.degree. to give 8.5 g. VIII acetate, m. 104-6.degree.. A soln. of 8.7 g. VIII acetate in 200 ml. 70% aq. HOAc is heated to 100.degree., 13.1 g. Zn dust is added in 5 min., and the mixt. is kept 50 min. at 100.degree. to give 5.3 g. 7-methoxy-3-phenylchroman-4-one (IX), m. 78-85.degree. (EtOH). A mixt. of

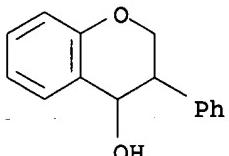
4 g. IX, 100 ml. tetrahydrofuran, and 1.2 g. LiAlH₄ is refluxed 5 hrs. to give 7-methoxy-3-phenylchroman-4-ol, m. 135-7.degree..

IT 1481-96-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 1481-96-5 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1967:28657 CAPLUS

DOCUMENT NUMBER: 66:28657

TITLE: 3,4-Diaryl-4-chromanols and 3,4-diaryl-3-chromenes

PATENT ASSIGNEE(S): Merck, E., A.-G.

SOURCE: Neth. Appl., 26 pp.

CODEN: NAXXAN

DOCUMENT TYPE: Patent

LANGUAGE: Dutch

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|-------|----------|-----------------|-------|
| NL 6517021 | ----- | 19660704 | ----- | ----- |

PRIORITY APPLN. INFO.: DE 19650102

GI For diagram(s), see printed CA Issue.

AB The title compds. are prep'd. by condensation of 3-aryl-4-chromanones with organo-metallic compds. followed by dehydration. A soln. of 0.66 g. I (R = R₁ = H) (IV) in 30 ml. abs. C₆H₆ is dropped to a soln. of p-MeOC₆H₄MgBr (from 2.2 g. p-MeOC₆H₄Br and 0.23 g. Mg) in abs. Et₂O, the Et₂O distd., and the mixt. refluxed 16 hrs., cooled, decompd. with 100 ml. 10% HCl, and the C₆H₆ layer sped. to yield II (R = R₁ = H, R₂ = MeO), m. 144-5.degree. (CHCl₃-Et₂O). Likewise, the following II are prep'd. (R, R₁, R₂, and m.p. given): H, H, H, 127-31.degree. (V); Et, H, H, 121-3.degree.; H, MeO, H, 151-2.degree.; Et, MeO, H, 158.degree. and 105.degree. (2 isomers); Et, MeO, MeO, 105-6.degree.; H, H, PhCH₂O, 122-3.degree. (VI); Et, MeO, PhCH₂O, 126.degree. and 137.degree. (2 isomers). To a soln. of IV (0.68 g.) in 30 ml. abs. C₆H₆ is added dropwise a soln. of PhLi (4 millimoles) in Et₂O. After the same treatment as above V is isolated; when the mixt. is heated 5 hrs. after adding 10% HCl, III (R = R₁ = R₂ = H) is obtained, m. 130-2.degree. (Et₂O-petroleum ether). Similarly prep'd. are III (R = R₁ = H, R₂ = MeO), m. 119-21.degree., and III (R = H, R₁ = R₂ = MeO), m. 162-5.degree.. By treating I [R = H, R₁ = tetrahydropyranyl-2-oxy (Q)] with PhMgBr as described, but decompg. with NH₄Cl soln., II (R = R₂ = H, R₁ = Q) is obtained, while from the alk. washing fluid some II (R = R₂ = H, R₁ = OH) (VIII) is isolated. Similarly is prep'd. from IV and p-QC₆H₄MgBr II (R = R₁ = H, R₂ = Q) (IX). VII (2 g.) is refluxed 2.5 hrs. in 50 ml. 5% HCl in dil. EtOH, the mixt. cooled and extd. with CHCl₃ to yield III (R = R₂ = H, R₁ = OH) (X); similarly are obtained III (R = R₁ = H, R₂ = OH) (XI), m. 188-9.degree., from IX, and III (R = H, R₁ = MeO, R₂ = OH), m. 118.degree.. A soln. of 2 g. VI in 200 ml. EtOAc is

hydrogenated at room temp. over 5% Pd-C, filtered, concd., the residue chromatographed on SiO₂, and eluted with C₆H₆ to yield II (R = R₁ = H, R₂ = OH) (XII); similarly are prep'd. II (R = H, R₁ = MeO, R₂ = OH), m. 173.degree. and II (R = Et, R₁ = MeO, R₂ = OH), m. 112.degree. and 150-2.degree. (2 isomers). XII (0.99 g.) is heated 5 hrs. at 100.degree. with a mixt. of 0.7 ml. H₂SO₄ and 13 ml. dioxane, cooled, poured on ice, extd. with CHCl₃, the ext. concd., and the residue crystd. from Et₂O-petroleum ether to give XI, m. 188-9.degree.. X (0.5 g.) in 10 ml. Me₂CO is boiled 24 hrs. in N with 0.3 g. ClCH₂CO₂Et and 0.35 g. anhyd. K₂CO₃, concd., and extd. with CH₂Cl₂ to yield III (R = R₂ = H, R₁ = EtO₂CCH₂O) (XIII). XI (1 g.), 4 g. 2-pyrrolidinonethyl chloride, 1.2 g. dry K₂CO₃, and 40 ml. abs. Me₂CO are stirred and boiled 20 hrs., concd., the residue dild. with H₂O and Et₂O, the Et₂O layer sepd. dried, on KOH, concd., and the residue chromatographed on Al₂O₃ and eluted with CHCl₃ to give III (R = R₁ = H, R₂ = 2-pyrrolidinoethoxy), m. 98-9.degree. (Me₂CO-Et₂O). X (1 g.), 5 ml. C₅H₅N, and 5 ml. Ac₂O are heated 5 hrs. at 50.degree., cooled, and extd. with CHCl₃ to yield III (R = R₂ = H, R₁ = AcO). To a soln. of 21 ml. POCl₃ in 210 ml. abs. C₅H₅N is added with stirring in 15 min. at 5.degree. a soln. of 7.8 g. X in 105 ml. C₅H₅N; after 15 hrs. at room temp. the mixt. is poured on a mixt. of 3 kg. ice and 300 ml. concd. HCl, heated at 100.degree. for 90 min., cooled, extd. with EtOAc, the ext. washed with HCl, dried on Na₂SO₄, filtered, and concd. to yield the phosphate of X. H₂NSO₃H (6 g.) and 7.5 g. X are suspended in 5 ml. abs. C₅H₅N, stirred 90 min. at 100.degree., cooled, filtered, the filter washed with C₅H₅N, the filtrate extd. with abs. Et₂O, the residue dried in vacuo, 75 ml. 12% NaOH and 53 ml. C₅H₅N added and shaken for 5 min.; the upper C₅H₅N layer washed with Et₂O, MeOH added and concd., and the residue crystd. from MeOH to yield III (R = R₂ = H, R₁ = OSO₃Na). XIII (2 g.) is refluxed 3 hrs. with 30 ml. 2N KOH in EtOH, and the soln. acidified to yield III (R = R₂ = H, R₁ = HO₂CCH₂O); XIII (3.5 g.) is refluxed 6 hrs. in a mixt. of 2 g. pyrrolidine and 10 ml. abs. C₆H₆, and the soln. concd. to yield III (R = R₂ = H, R₁ = QCOCH₂O) (Q = pyrrolidino). II and III have antigenadotropic and contraceptive effects.

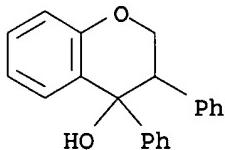
IT 13417-62-4P 13417-63-5P 13417-67-9P

13619-77-7P 13619-78-8P 13620-06-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

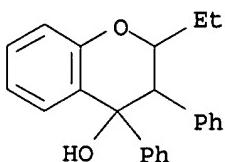
RN 13417-62-4 CAPLUS

CN 4-Chromanol, 3,4-diphenyl- (8CI) (CA INDEX NAME)



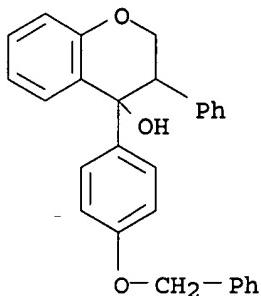
RN 13417-63-5 CAPLUS

CN 4-Chromanol, 2-ethyl-3,4-diphenyl- (8CI) (CA INDEX NAME)



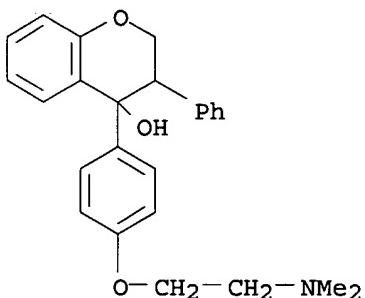
RN 13417-67-9 CAPLUS

CN 4-Chromanol, 4-[p-(benzylloxy)phenyl]-3-phenyl- (8CI) (CA INDEX NAME)



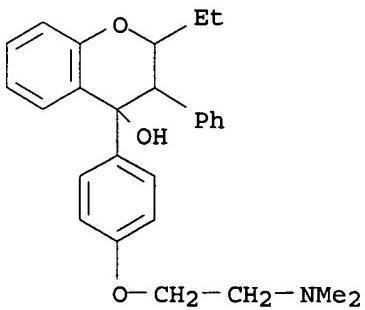
RN 13619-77-7 CAPLUS

CN 4-Chromanol, 4-[p-[2-(dimethylamino)ethoxy]phenyl]-3-phenyl- (8CI) (CA INDEX NAME)



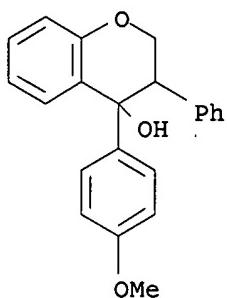
RN 13619-78-8 CAPLUS

CN 4-Chromanol, 4-[p-[2-(dimethylamino)ethoxy]phenyl]-2-ethyl-3-phenyl- (8CI) (CA INDEX NAME)



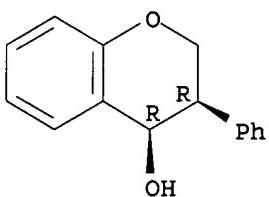
RN 13620-06-9 CAPLUS

CN 4-Chromanol, 4-(p-methoxyphenyl)-3-phenyl- (8CI) (CA INDEX NAME)



L4 ANSWER 21 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1966:35186 CAPLUS
 DOCUMENT NUMBER: 64:35186
 ORIGINAL REFERENCE NO.: 64:6453c-d
 TITLE: Nuclear magnetic resonance of .alpha.-epoxy ketones
 AUTHOR(S): Pierre, Jean Louis; Chautemps, Pierre; Arnaud, Paul
 CORPORATE SOURCE: Fac. Sci., Grenoble, Fr.
 SOURCE: Compt. Rend. (1965), 261(20(Groupe 6)), 4025-7
 DOCUMENT TYPE: Journal
 LANGUAGE: French
 GI For diagram(s), see printed CA Issue.
 AB The configuration of a series of .alpha.-epoxy ketones (I, R = H, Me, R1 = H, Me, iso-Pr, tert-Bu, neopentyl, R2 = Me and 3,3-dimethyl-2-oxiranyl) was established by N.M.R. The conformation of the Ac group was also detd.
 IT 6212-70-0, 4-Isoflavanol, cis-
 (nuclear magnetic resonance of)
 RN 6212-70-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



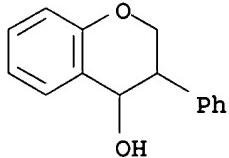
L4 ANSWER 22 OF 23 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1964:432298 CAPLUS
 DOCUMENT NUMBER: 61:32298
 ORIGINAL REFERENCE NO.: 61:5601g-h,5602a-b
 TITLE: Synthetic isoflavones. VI. The reaction of isoflavan-4-ols with acetic acid
 AUTHOR(S): Inoue, Naoto
 CORPORATE SOURCE: Tohoku Univ., Sendai
 SOURCE: Bull. Chem. Soc. Japan (1964), 37(5), 606-9
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 GI For diagram(s), see printed CA Issue.
 AB Treatment of 500 mg. I, (R = OMe, R = H, X = OH), (.beta.-isomer) (III)

with 10 ml. HOAc at reflux 1 hr. gave 300 mg. II, (R = OMe, R' = H), (IV), m. 108.degree. (EtOH). Treatment of 100 mg. III with 10 ml. HOAc at 50.degree. 1 hr. gave 70 mg. I, (R = OMe, R' = H, X = OAc) (.alpha.-isomer) (V). Reaction of 50 mg. I, (R = OMe, R' = H, X = OH) (.alpha.-isomer) (VI) with 5 ml. HOAc at reflux. 1 hr. gave 55 mg. IV, and at 50.degree. in HOAc 1 hr., VI gave V. Reaction of 100 mg. I, (R = OMe, R' = H, X = OAc) (.beta.-isomer) (VII) in 10 ml. HOAc at reflux 1 hr. gave IV. At 50.degree. 1 hr., 100 mg. VII in 10 ml. HOAc gave 55 mg. V. Reaction of 100 mg. V in 10 ml. HOAc at reflux 1 hr. gave 70 mg. IV. Treatment of 100 mg. VII with 1.0 ml. 0.5N NaOMe in 20 ml. MeOH at room temp. 24 hrs. gave 60 mg. III. Treatment of 50 mg. V with 0.5 ml. 0.5N NaOMe in 20 ml. MeOH at room temp. 12 hrs. gave 28 mg. VI. Addn. of 2 drops concd. H₂SO₄ or HCl to 50 mg. III in 40 ml. 1: 1 H₂O-dioxane and allowing the mixt. to stand at room temp. 48 hrs. gave 20 mg. VI. Treatment of 50 mg. I, (R = R' = H, X = OH) with 10 ml. HOAc at 50.degree. 1 hr. gave no reaction. Reaction of 50 mg. I, (R = R' = OMe, X = OH) (VIII) with 10 ml. HOAc at 50.degree. 1 hr. gave 20 mg. II, (R = R' = OMe) (IX). Treatment of 100 mg. VIII with 10 ml. HOAc at 50.degree. 1 hr. gave 30 mg. C₁₉H₂₀O₅, m. 123.degree.. In 20 ml. boiling HOAc 1 hr., 100 mg. VIII gave 60 mg. IX. Redn. of 500 mg. IV in 140 ml. HOAc with H over 500 mg. 20% Pd-C at 30.degree. gave 300 mg. I, (R = OMe, R' = X = H). Redn. of 500 mg. IX in 150 ml. HOAc with H over 1.0 g. 5% Pd-C at 20.degree. gave 200 mg. I, (R = R' = OMe, X = H), (X), m. 114.degree. (EtOH). Redn. of 250 mg. 7,4'-dimethoxyisoflavone with 3.6 g. Zn(Hg) and 5 ml. concd. HCl in 30 ml. HOAc at room temp. 24 hrs. gave 150 mg. X. The .alpha.-series is believed to be trans- and the .beta.-series cis.

IT 1481-96-5, 4-Isoflavanol
(derivs., reaction with HAc)

RN 1481-96-5 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 23 OF 23 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1964:432297 CAPLUS

DOCUMENT NUMBER: 61:32297

ORIGINAL REFERENCE NO.: 61:5601c-g

TITLE: Synthetic isoflavones. V. The reduction of isoflavones

AUTHOR(S): Inoue, Naoto

CORPORATE SOURCE: Tohoku Univ., Sendai

SOURCE: Bull. Chem. Soc. Japan (1964), 37(5), 601-5

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

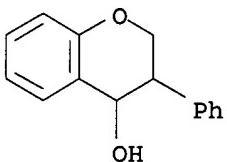
AB cf. CA 58, 5619b. Various methods of redn. of isoflavones (I) gave different products and different stereochem. results. Redn. of 0.5 g. I, (R = R' = H), (III) in 100 ml. EtOH with 1 atm. H over 0.5 g. Raney Ni 80 min. at 28.degree. gave 0.38 g. II, (R = R' = H, X = OH), (IV), m. 75.degree. (petr. ether). Treatment of 0.2 g. IV with 2 ml. Ac₂O and 1 ml. C₅H₅N 20 hrs. at room temp. gave apprx. 100% II, (R = R' = H, X = OAc) m. 93.degree. (petr. ether). Redn. of 1.0 g. III in 40 ml. HOAc over 0.2 g. PtO₂ with H at 28.degree. 28 min. gave 0.7 g. IV. A mixt. of 1.0 g. III, 3.7 g. Al (O iso-Pr)₃, and 40 ml. of iso-PrOH was heated at

100.degree. 1.5 hrs. to give 0.8 g. IV. Redn. of 1.0 g. III with (1 atm.) H over 0.3 g. 10% Pd-C in 100 ml. EtOH gave 0.75 g. II, (R = R' = X = H), (V), m. 55.degree. (EtOH). Reaction of 5 ml. concd. HCl, 0.3 g. III, and 0.5 g. Zn(Hg) in 20 ml. HOAc 24 hrs. at room temp. gave 0.22 g. V. Redn. of 1.0 g. I, (R = OMe, R' = H), (VI) with (1 atm.) H over 1.2 g. Raney Ni in 60 ml. EtOH at 20.degree. 4 hrs. gave 0.4 g. II, (R = OMe, R' = H, X = OH), (VII), .beta.-isomer, m. 144.degree. (EtOH). Treatment of VII with Ac₂O and C₅H₅N at room temp. gave II, (R = OMe, R' = H, X = OAc), .beta.-isomer, m. 121.degree. (EtOH). A soln. of 1.0 g. VI and 2.5 g. Al(O iso-Pr)₃ in 30 ml. iso-PrOH on heating 1 hr. gave 0.65 g. VII. Reaction of 1.5 g. VI with 3.0 g. Al(O iso-Pr)₃ in 65 ml. iso-PrOH 4.5 hrs. at reflux gave 0.9 g. VII and 0.2 g. II, (R = OMe, R' = H, X = O iso-Pr), m. 111.degree.. Treatment of 10.0 g. VI with 1.2 g. NaBH₄ in 600 ml. EtOH at 36.degree. 2 days gave 4.5 g. VII and 2.2 g. II, (R = OMe, R' = H, X = OH), (VIII), .alpha.-isomer, m. 131.degree. (EtOH). Treatment of VIII with Ac₂O and C₅H₅N at room temp. gave II, (R = OMe, R' = H, X = OAc), .alpha.-isomer, m.p. 111.degree. (EtOH). Redn. of 0.5 g. VI with H over 0.3 g. 10% Pd-C in 40 ml. HOAc at 24.degree. 37 min. gave 0.25 g. II, (R = OMe, R' = X = H), (IX), m. 105-6.5.degree.. Reaction of 0.5 g. VI with 10 ml. concd. HCl and 10 g. Zn(Hg) in 30 ml. HOAc 24 hrs. at room temp. gave 0.3 g. IX. Redn. of 0.5 g. I, (R = R' = OMe), (X) with H₂ over Raney Ni (from 2.0 g. alloy) in 200 ml. EtOH at 19.degree. 1 hr. gave 0.31 g. II, (R = R' = OMe, X = OH), (XI), m. 143.degree. (EtOH). Treatment of 1.0 g. .times. with 0.1 g. NaBH₄ in 450 ml. EtOH at 15.degree. 2 days gave 0.5 g. XI. Reaction of 1.0 g. .times. with 0.7 g. Al(O iso-Pr)₃ and 40 ml. iso-PrOH 1 hr. at reflux gave 0.6 g. XI. Reaction of 2.0 g. X, 2.0 g. Al(O iso-Pr)₃, and 240 ml. isoPrOH at reflux 10 hrs. gave 1.2 g. II, (R = R' = OMe, X = O Pr-iso), m. 75.5.degree. (EtOH) and 0.05 g. 7,4'-dimethoxyisoflav-3-ene, m. 161.degree. (petr. ether). It is thought that the .beta.-isomers (VII) are cis and that the .alpha.-isomers (VIII) are trans.

IT 1481-96-5, 4-Isoflavanol
(prepn. of)

RN 1481-96-5 CAPLUS

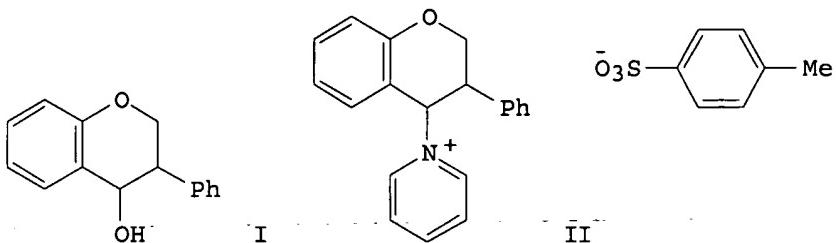
CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 16 tot

L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1980:215213 CAPLUS
DOCUMENT NUMBER: 92:215213
TITLE: Syntheses of isoflavan-4-(1-pyridinium) salts
AUTHOR(S): Szabo, Vince; Borbely, Janos; Antal, Erno
CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Lajos Univ., Debrecen,
H-4010, Hung.
SOURCE: Acta Chim. Acad. Sci. Hung. (1979), 102(1), 51-7
CODEN: ACASA2; ISSN: 0001-5407
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



AB Treatment of trans(.alpha.)- or cis(.beta.)-4-hydroxyisoflavan (I) with p-MeC₆H₄SO₂Cl in pyridine gives, instead of the expected tosylates, the same isoflavan-4-(1-pyridinium) tosylate (II). The anion of II is exchangeable for other anions. Reductive methods convert II to isoflavin and 4-[1-(1,4-dihydropyridyl)]isoflavan; in alk. medium it can be converted to isoflav-3-ene.

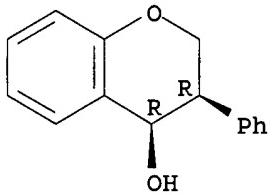
IT 6212-70-0P 20986-77-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prep. and reaction with toluenesulfonyl chloride and pyridine)

RN 6212-70-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

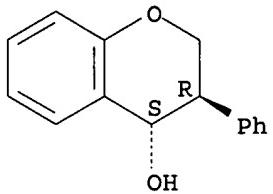
Relative stereochemistry.



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

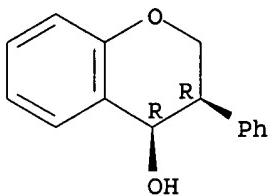
Relative stereochemistry.



L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1977:120467 CAPLUS

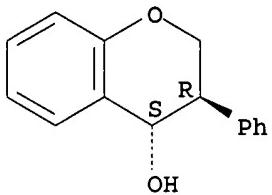
DOCUMENT NUMBER: 86:120467



RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1969:11493 CAPLUS

DOCUMENT NUMBER: 70:11493

TITLE: Syntheses of trans-isoflavan-4-ols

AUTHOR(S): Yamaguchi, Shozo; Ito, Shoei; Suzuki, Ikuko; Inoue, Naoto

CORPORATE SOURCE: Tohoku Univ., Sendai, Japan

SOURCE: Bull. Chem. Soc. Jap. (1968), 41(9), 2073-7

CODEN: BCSJA8

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The reaction of nitrous acid and three 4-aminoisoflavan hydrochlorides (I, II, and III) obtained by the catalytic **hydrogenation** of isoflavanone oximes, and the hydroboration of 3 isoflavenes (IV, V, and VI), were investigated in the hope of finding a general method of synthesizing trans-isoflavan-4-ols. The reaction of I and II with nitrous acid afforded the corresponding trans-4-ols, though in a poor yield, but that of III produced no expected compd., the corresponding isoflavene VI being obtained instead. The hydroboration of IV, V, and VI afforded the corresponding trans-alcs. (VII, VIII, and IX) in good yields. In addn., it became clear that 4-aminoisoflavans obtained by the catalytic redn. of the oximino compds. possess the 3,4-cis configuration.

IT 20986-77-0P

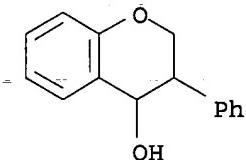
RL: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)

RN 20986-77-0 CAPLUS

CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

TITLE: Reductive conversions of chromanoids. I. Catalytic
 hydrogenation of isoflavone (3-phenylchromone)
 AUTHOR(S): Szabo, Vince; Antal, Erno
 CORPORATE SOURCE: Dep. Appl. Chem., Kossuth Lajos Univ., Debrecen, Hung.
 SOURCE: Acta Chim. Acad. Sci. Hung. (1976), 90(4), 381-93
 CODEN: ACASA2
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A kinetic study of the **hydrogenation** of isoflavone over a Pd/C catalyst showed that the rate and the product distribution are dependent upon the solvent, pH of the soln., and the activity of the catalyst. Selective **hydrogenation**, by appropriate choice of conditions, gave predominantly isoflavanone, 4-isoflavanol, isoflavan, or, in dil. alkali, 2-hydroxy-.alpha.-methyldeoxybenzoin.
 IT 1481-96-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 RN 1481-96-5 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl- (9CI) (CA INDEX NAME)



(AD241-T42)

~~QD481-T44~~

L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1973:491915 CAPLUS
 DOCUMENT NUMBER: 79:91915
 TITLE: Selective reduction of isoflavone
 AUTHOR(S): Szabo, Vince; Antal, Erno
 CORPORATE SOURCE: Inst. Appl. Chem., Kossuth Univ., Debrecen, Hung.
 SOURCE: Tetrahedron Lett. (1973), (19), 1659-62
 CODEN: TELEAY
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI For diagram(s), see printed CA Issue.
 AB Isoflavone (I) with Pd-H in EtOH or dioxane gave isoflavan-4-ol (II, R = H, OH) and isoflavanone (II, R = O), resp., almost quant. The effect of pH on the **hydrogenation** of I in buffered aq. EtOH was studied and thereby 90% II (R = O) was obtained by stopping the reaction after the absorption of 1 mole of H. At pH 11.5 2-HOC₆H₄COCHRPh (R = H and Me) was formed.
 IT 6212-70-0P 20986-77-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 RN 6212-70-0 CAPLUS
 CN 2H-1-Benzopyran-4-ol, 3,4-dihydro-3-phenyl-, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.